## Scientific and Technical Information Center

## SEARCH REQUEST FORM

equester's Full Name: MARK BERCH Examiner #: 59193 Date: 5/9/05
rt Unit: 1624 Phone Number: 2-0663 Serial Number: (063404)  ocation (Bldg/Room#): 5 COI (Mailbox #): 5 CI8 Results Format Preferred (circle): PAPER DISK  ***********************************
ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following:
tle of Invention:
ventors (please provide full names):
arliest Priority Date:
arch Topic:  ease provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the extending species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. If the any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.
For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the propriate serial number. $ \begin{pmatrix} H   C_{1} + \alpha   Kyk \end{pmatrix} $ $ \begin{pmatrix} H   C_{1} + \alpha   Kyk \end{pmatrix} $ $ \begin{pmatrix} R^{3} \\ K = 1 - 3 \end{pmatrix} $ $ \begin{pmatrix} H   C_{1} + \alpha   Kyk \end{pmatrix} $ $ \begin{pmatrix} R^{1} \\ K = 1 - 3 \end{pmatrix} $ $ \begin{pmatrix} H   C_{1} + \alpha   Kyk \end{pmatrix} $ $ \begin{pmatrix} H   C$
$T = -N \left( \frac{1}{\sqrt{1 - 4}} \right) N + C$
$\frac{1}{2} = \frac{C NH_{2} N-c-0 H}{m=0-4}$ $\frac{1}{2} = \frac{1}{4} \frac{ C N OC 05C}{m=0-4}$
$= H(C/N) OC 100C$ not in ring $(H_2)_n n = 200$ 2-10
$\frac{3}{2} = \frac{1}{2} \left( \frac{1}{2} + \frac{1}{2} \right) \left( \frac{1}{2} + \frac{1}{2} + \frac{1}{2} \right) \left( \frac{1}{2} + \frac{1}{$
= -N set con nationing   N Cn N - J-C' - N N - C' - N
Can't be honzerd  Ning  Ci-N  -(C)  CK  CK

111 Page Blank (uspto)

=> fil reg; d stat que 129; fil capl uspatf toxcenter; s 129 FILE 'REGISTRY' ENTERED AT 16:36:06 ON 12 MAY 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 11 MAY 2005 HIGHEST RN 850303-40-1 DICTIONARY FILE UPDATES: 11 MAY 2005 HIGHEST RN 850303-40-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

s— C @23 24

VAR G1=C/NH2/26/H
VAR G2=H/C/N/20/22/23
VAR G3=O/S
NODE ATTRIBUTES:
NSPEC IS RC AT 13
CONNECT IS E1 RC AT 22
DEFAULT MLEVEL IS ATOM

-full file search done on athis structure

0 @22

## DEFAULT ECLEVEL IS LIMITED

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GRAPH ATTRIBUTES:
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RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 27

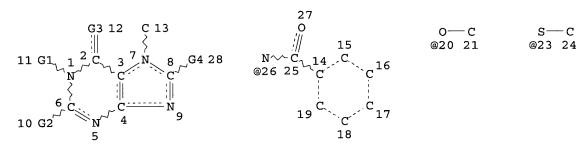
STEREO ATTRIBUTES: NONE

L12

35177 SEA FILE=REGISTRY SSS FUL L9

L20

STR



C @29 N@30

 $N \sim G6 \sim N$ @31 32 33

CH~ G5 \rightarrow Cb @34 35 36 N-√G7 √ Cb @37 38 39

our constant was purple for the

VAR G1=C/NH2/26/H

VAR G2=H/C/N/20/23

VAR G3=0/S

VAR G4=29/30/31/34/37/40/48

REP G5 = (0-3) CH

REP G6 = (1-4) CH

REP G7 = (0-4) CH

REP G8 = (0-2) CH

REP G9=(1-3) C

NODE ATTRIBUTES:

NSPEC IS RC AT13

NSPEC IS R AT29

IS R NSPEC

AT 30

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

## GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 47

STEREO ATTRIBUTES: NONE

L22

456 SEA FILE=REGISTRY SUB=L12 SSS FUL L20

L24

STR

Page 1-A CH-G15~G5 @88 89 90

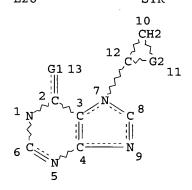
Page 2-A VAR G3=0/SVAR G4=56/59/60/65/70/75/48/83/84/88 VAR G5=NH2/49/52 REP G6=(1-9) C REP G8 = (0-2) CH REP G9=(1-3) C REP G10=(2-10) C REP G11 = (0-4) C REP G12 = (0-3) C REP G13=(1-4) CH REP G14=(0-1) CH REP G15 = (1-3) CH NODE ATTRIBUTES: NSPEC IS RC AΤ 13 CONNECT IS E1 RC AT 50 CONNECT IS E1 RC AT 51 CONNECT IS E1 RC AT 53 DEFAULT MLEVEL IS ATOM **GGCAT** IS SAT AT67 **GGCAT** IS SAT AT 72

GRAPH ATTRIBUTES:

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DEFAULT ECLEVEL IS LIMITED

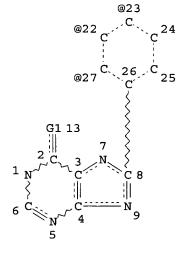
STEREO ATTRIBUTES: NONE L26 STR



VAR G1=O/S REP G2=(1-9) CH2 NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE L27 STR



G2 @28

VAR G1=O/S
VAR G2=NH2/14/17/19
REP G3=(0-3) C
VAR G5=NH2/14/17
VPA 28-22/27/23 U
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 15
CONNECT IS E1 RC AT 16
CONNECT IS E1 RC AT 18

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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE

L29 445 SEA FILE=REGISTRY SUB=L22 SSS FUL (L24 NOT (L26 OR L27))

100.0% PROCESSED 456 ITERATIONS 445 ANSWERS

SEARCH TIME: 00.00.01

FILE 'CAPLUS' ENTERED AT 16:36:06 ON 12 MAY 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'USPATFULL' ENTERED AT 16:36:06 ON 12 MAY 2005
CA INDEXING COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'TOXCENTER' ENTERED AT 16:36:06 ON 12 MAY 2005 COPYRIGHT (C) 2005 ACS

L31 22 L29

=> dup rem 131

PROCESSING COMPLETED FOR L31

L32 17 DUP REM L31 (5 DUPLICATES REMOVED)

ANSWERS '1-12' FROM FILE CAPLUS ANSWERS '13-17' FROM FILE USPATFULL

=> d ibib ed abs hitstr 1-17; fil hom

L32 ANSWER 1 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN DUPLICATE 1

ACCESSION NUMBER:

2003:991509 CAPLUS

DOCUMENT NUMBER:

140:42192

TITLE:

SOURCE:

Preparation of purinone derivatives as

dipeptidylpeptidase IV (DPP-IV) inhibitors

INVENTOR(S):

Yoshikawa, Seiji; Emori, Eita; Matsuura, Fumiyoshi;

Richard, Clark; Ikuta, Hironori; Kira, Kazunobu;

Yasuda, Nobuyuki; Nagakura, Tadashi; Yamazaki, Kazuto

PATENT ASSIGNEE(S):

IGNEE (2):

Eisai Co., Ltd., Japan PCT Int. Appl., 376 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.			KIND		DATE		APPLICATION NO.						DATE		
WO 2003104229			 λ1		20021219		WO 2003-JP7010						20020603		
	AE, AG,												_		
и.	CO, CR,	•	•	•	•	•	•	•	•	•	•	•	•	•	•
	GM, HR,		-	•	•		•						•	•	•

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LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH,
             PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
    EP 1514552
                          A1
                                20050316
                                           EP 2003-733276
                                                                    20030603
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
    BR 2003011697
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    NS 2004116328
                                20040617
                                            US 2003-457002
                          Α1
                                                                    20030606
PRIORITY APPLN. INFO .:
                                            JP 2002-166069
                                                                 A 20020606
                                            JP 2002-209373
                                                                 A 20020718
                                            JP 2002-307750
                                                                 Α
                                                                    20021023
                                            WO 2003-JP7010
                                                                 W
                                                                    20030603
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OTHER SOURCE(S): MARPAT 140:42192

Ι

ED Entered STN: 21 Dec 2003

GT

AB The title compds. I [wherein T1 is an optionally substituted, monocyclic or bicyclic, 4- to 12-membered, heterocyclic group containing one or two nitrogen atoms in the ring; X is optionally substituted C1-6 alkyl, etc.; Z1 and Z2 each independently is nitrogen, CR2; and R1 and R2 each independently is hydrogen, optionally substituted C1-6 alkyl, optionally substituted C1-6 alkoxy, etc.] are prepared Compds. of this invention in vitro showed IC50 values of 0.001 μM to 1.48 μM against dipeptidylpeptidase IV.

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635715-41-2P 635715-43-4P 635715-48-9P
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     635715-64-9P 635715-66-1P 635715-68-3P
     635715-79-6P 635715-81-0P 635715-83-2P
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    RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of purinone derivs. as dipeptidylpeptidase IV inhibitors)
RN
     635715-41-2 CAPLUS
     Acetic acid, [[7-(2-chlorophenyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-
CN
     piperazinyl)-1H-purin-2-yl]oxy]-, ethyl ester, mono(trifluoroacetate)
     (9CI) (CA INDEX NAME)
     CM
          1
```

CRN 635715-40-1 CMF C20 H23 Cl N6 O4

CM 2

RN 635715-43-4 CAPLUS

CN Acetic acid, [[7-(2-chlorophenyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]oxy]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-42-3 CMF C18 H19 Cl N6 O4

$$\begin{array}{c|c} H & \\ H & \\ N & \\ N & \\ N & \\ Me & \\ O & \\ C1 & \\ \end{array}$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635715-48-9 CAPLUS

CN Benzeneacetic acid, α-[[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]oxy]-, methyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-47-8 CMF C23 H26 N6 O4

CRN 76-05-1 CMF C2 H F3 O2

RN 635715-52-5 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-(1-methylpropoxy)-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-51-4 CMF C18 H26 N6 O2

$$\begin{array}{c|c} \text{Me} & & & \\ \text{Et-CH-O} & \text{N} & \text{N} & \\ \text{Me} & & \text{N} & \\ \text{O} & & \text{CH}_2\text{-}\text{C} \end{array} \subset \text{Me} \\ \end{array}$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635715-57-0 CAPLUS

CN Butanoic acid, 2-[[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]oxy]-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-56-9 CMF C20 H28 N6 O4

EtO-
$$C$$
Et- $CH-O$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $CH_2-C$ 
 $C-Me$ 

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635715-58-1 CAPLUS

CN Propanoic acid, 2-[[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]oxy]-, ethyl ester (9CI) (CA INDEX NAME)

RN 635715-60-5 CAPLUS

CN Propanoic acid, 2-[[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]oxy]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-59-2 CMF C17 H22 N6 O4

$$\begin{array}{c|c} \text{Me} & & & \text{NH} \\ \text{HO}_2\text{C-CH-O} & & & \text{N} \\ \text{Me} & & & \text{N} \\ \text{O} & & & \text{CH}_2\text{-C} \\ \end{array} \begin{array}{c} \text{NH} \\ \text{CH}_2\text{-C} \\ \end{array}$$

CRN 76-05-1 CMF C2 H F3 O2

RN

635715-62-7 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-2-methoxy-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-61-6 CMF C15 H20 N6 O2

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635715-63-8 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-2-ethoxy-1,7-dihydro-1-methyl-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)

EtO N N N N N N N N 
$$\sim$$
 CH<sub>2</sub>-C $\Longrightarrow$  C-Me

RN 635715-64-9 CAPLUS

CN Acetic acid, [[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]oxy]-, ethyl ester (9CI) (CA INDEX NAME)

RN 635715-66-1 CAPLUS

CN Acetic acid, [[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]oxy]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-65-0 CMF C16 H20 N6 O4

CM 2

RN 635715-68-3 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-2-(2-methoxyethoxy)-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-67-2 CMF C17 H24 N6 O3

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635715-79-6 CAPLUS

CN 1H-Purine-2-acetic acid, 7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-78-5 CMF C18 H24 N6 O3

EtO-C-CH<sub>2</sub>
N
N
N
N
$$CH_2$$
-C=C-Me

CM 2

RN 635715-81-0 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1,2-dimethyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-80-9 CMF C15 H20 N6 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635715-83-2 CAPLUS

CN 6H-Purin-6-one, 2-butyl-7-(2-butynyl)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-82-1 CMF C18 H26 N6 O

CRN 76-05-1 CMF C2 H F3 O2

RN 635715-85-4 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-(phenylmethyl)-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-84-3 CMF C21 H24 N6 O

Ph-CH<sub>2</sub> N N N N N N N N N N 
$$\sim$$
 CH<sub>2</sub>-C $\Longrightarrow$  C-Me

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635715-87-6 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-(2-phenylethyl)-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-86-5 CMF C22 H26 N6 O

CRN 76-05-1 CMF C2 H F3 O2

RN 635715-91-2 CAPLUS

CN 6H-Purin-6-one, 2-amino-7-(2-butynyl)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-90-1 CMF C14 H19 N7 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635715-93-4 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-(methylamino)-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 635715-92-3 CMF C15 H21 N7 O

MeNH N N N N N 
$$CH_2-C$$
  $C=C-Me$ 

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635715-95-6 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-2-(dimethylamino)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-94-5 CMF C16 H23 N7 O

CM 2

RN 635715-97-8 CAPLUS

CN Glycine, N-[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-96-7 CMF C18 H25 N7 O3

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635715-99-0 CAPLUS

CN Glycine, N-[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-98-9 CMF C16 H21 N7 O3

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-01-7 CAPLUS

CN Glycine, N-[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]-N-methyl-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-00-6 CMF C19 H27 N7 O3

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-05-1 CAPLUS

CN Glycine, N-[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]-N-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-04-0 CMF C17 H23 N7 O3

$$\begin{array}{c|c} \text{Me} & & \text{NH} \\ \text{HO}_2\text{C}-\text{CH}_2-\text{N} & & \text{N} \\ & & \text{N} & & \text{N} \\ \text{Me} & & \text{N} & & \text{N} \\ & & & \text{CH}_2-\text{C} \end{array}$$

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-09-5 CAPLUS

CN Alanine, N-[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]-, methyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-08-4 CMF C18 H25 N7 O3

MeO-C-CH-NH N N NH
Me 
$$\sim$$
 CH<sub>2</sub>-C= C-Me

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-11-9 CAPLUS

CN Alanine, N-[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-

purin-2-yl]-2-methyl-, methyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-10-8 CMF C19 H27 N7 O3

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-13-1 CAPLUS
CN L-Alanine, N-[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)1H-purin-2-yl]-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-12-0 CMF C19 H27 N7 O3

Absolute stereochemistry.

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-15-3 CAPLUS

CN L-Alanine, N-[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-14-2 CMF C17 H23 N7 O3

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-17-5 CAPLUS

CN β-Alanine, N-[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]-, ethyl ester, mono(trifluoroacetate) (9CI)
 (CA INDEX NAME)

CM 1

CRN 635716-16-4 CMF C19 H27 N7 O3

$$\begin{array}{c|c} O \\ \parallel \\ E \text{to-} \text{C-} \text{CH}_2 - \text{CH}_2 - \text{NH} \\ \text{Me} \\ \hline \\ N \\ \text{N} \\ N \\ \text{N} \\ N \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{CH}_2 - \text{C} \\ \text{C-} \text{Me} \\ \end{array}$$

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-19-7 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-2-[(2-ethoxyethyl)amino]-1,7-dihydro-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-18-6 CMF C18 H27 N7 O2

EtO-
$$CH_2$$
- $CH_2$ - $NH$ 

N

N

N

 $CH_2$ - $C$ 
 $C$ 
 $C$ 
 $C$ 

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-23-3 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-[(phenylmethyl)amino]-

8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-22-2 CMF C21 H25 N7 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-27-7 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-[methyl(phenylmethyl)amino]-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-26-6 CMF C22 H27 N7 O

CM 2

RN 635716-29-9 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-2-[[(4-chlorophenyl)methyl]amino]-1,7-dihydro-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-28-8 CMF C21 H24 Cl N7 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-31-3 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-2-[[(4methoxyphenyl)methyl]amino]-1-methyl-8-(1-piperazinyl)-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-30-2 CMF C22 H27 N7 O2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-33-5 CAPLUS
CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-[(2-phenylethyl)amino]-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-32-4 CMF C22 H27 N7 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-35-7 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-[methyl(2-phenylethyl)amino]-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-34-6 CMF C23 H29 N7 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-39-1 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-2-[(2-pyridinylmethyl)amino]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-38-0 CMF C20 H24 N8 O

CM 2

RN 635716-45-9 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-2-(diethylamino)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-44-8 CMF C18 H27 N7 O

Et<sub>2</sub>N N N N N N N N N N N 
$$\sim$$
 CH<sub>2</sub>-C $=$  C-Me

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-47-1 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-2-(ethylmethylamino)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-46-0 CMF C17 H25 N7 O

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-53-9 CAPLUS

CN Acetonitrile, [[7-(2-butynyl)-6,7-dihydro-1~methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]methylamino]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-52-8 CMF C17 H22 N8 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-55-1 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-[(1methylethyl)amino]-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA
INDEX NAME)

CM 1

CRN 635716-54-0 CMF C17 H25 N7 O

i-PrNH N N N N 
$$\sim$$
 NH  $\sim$  NH

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-57-3 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-2-(2-pyridinylamino)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-56-2 CMF C19 H22 N8 O

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-59-5 CAPLUS CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-(phenylamino)-8-(1piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-58-4 CMF C20 H23 N7 O

PhNH N N N NH 
$$\sim$$
 NH  $\sim$  NH  $\sim$  NH  $\sim$  CH<sub>2</sub>-C $\Longrightarrow$  C-Me

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-65-3 CAPLUS

N Alanine, N-[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-64-2 CMF C17 H23 N7 O3

$$\begin{array}{c|c} \text{Me} & & & \\ \text{HO}_2\text{C}-\text{CH}-\text{NH} & & & \\ \text{N} & & & \\ \text{Me} & & & \\ \end{array}$$

CM 2 -

RN 635716-67-5 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-2-(2-pyridinylmethoxy)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-66-4 CMF C20 H23 N7 O2

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-69-7 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-(1-methylethoxy)-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-68-6 CMF C17 H24 N6 O2

i-Pro N N N N N 
$$\sim$$
 NH  $\sim$  CH<sub>2</sub>-C $\Longrightarrow$  C-Me

CRN 76-05-1 CMF C2 H F3 O2

635716-71-1 CAPLUS RN

6H-Purin-6-one, 7-(2-butynyl)-2-(2-butynyloxy)-1,7-dihydro-1-methyl-8-(1-CNpiperazinyl) -, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM

635716-70-0 CRN CMF C18 H22 N6 O2

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN

635716-73-3 CAPLUS
Acetic acid, [[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-CN1H-purin-2-yl]thio]-, methyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM1

CRN 635716-72-2 CMF C17 H22 N6 O3 S

MeO-C-CH<sub>2</sub>-S
N
N
N
N
N
N
CH<sub>2</sub>-C
$$=$$
 C-Me

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-75-5 CAPLUS
CN Propanoic acid, 2-[[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]thio]-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-74-4 CMF C19 H26 N6 O3 S

CM 2

RN 635716-77-7 CAPLUS

CN Propanoic acid, 3-[[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]thio]-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-76-6 CMF C19 H26 N6 O3 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-79-9 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-2-(ethylthio)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-78-8 CMF C16 H22 N6 O S

Ets N N N N N N N N N N N 
$$\sim$$
 CH<sub>2</sub>-C $\Longrightarrow$  C-Me

CM 2

RN 635716-81-3 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-2-[(2-hydroxyethyl)thio]-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-80-2 CMF C16 H22 N6 O2 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-86-8 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-(methylthio)-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-85-7 CMF C15 H20 N6 O S

$$\begin{array}{c|c} \text{MeS} & \text{N} & \text{N} & \text{NH} \\ \hline \text{N} & \text{N} & \text{N} & \text{N} \\ \hline \text{Me} & \text{CH}_2-\text{C} \end{array} \subset \text{C-Me}$$

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-90-4 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-[(1-methylethyl)thio]-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-89-1 CMF C17 H24 N6 O S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-93-7 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-2-[(1,1-dimethylethyl)thio]-1,7-dihydro-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-92-6 CMF C18 H26 N6 O S

CRN 76-05-1 CMF C2 H F3 O2

RN 635717-00-9 CAPLUS

CN Acetic acid, [[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]thio]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-99-3 CMF C16 H20 N6 O3 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635717-02-1 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-2-(ethylsulfinyl)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 635717-01-0 CMF C16 H22 N6 O2 S

Et-S N N N N N N N N N N N 
$$CH_2-C \equiv C-Me$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635717-05-4 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-2-(ethylsulfonyl)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635717-04-3 CMF C16 H22 N6 O3 S

$$\begin{array}{c|c} O & & & & \\ \parallel & & & & \\ N & & & & \\ \hline O & N & & & \\ Me & & & & \\ O & & & & \\ \end{array}$$

CM 2

RN 635717-08-7 CAPLUS

CN 1H-Purine-2-carbonitrile, 7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635717-07-6 CMF C15 H17 N7 O

NC N N N N N N N N N N 
$$\sim$$
 CH<sub>2</sub>-C $\equiv$  C-Me

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635717-10-1 CAPLUS

CN 1H-Purine-2-carboxamide, 7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & & \\ H_2N-C & & N & & N \\ \hline & CH_2-C \Longrightarrow C-Me \\ \end{array}$$

RN 635717-13-4 CAPLUS

CN 1H-Purine-2-carboxylic acid, 7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 635717-12-3 CMF C15 H18 N6 O3

CM 2

CRN 76-05-1 CMF C2 H F3 O2

CN

RN 635717-16-7 CAPLUS

6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635717-15-6 CMF C14 H18 N6 O

CM 2

RN 635717-18-9 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-2-methoxy-1-(2-phenylethyl)-8-(1-piperazinyl)-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{MeO} & \text{N} & \text{N} & \text{NH} \\ \text{Ph-CH}_2-\text{CH}_2 & \text{CH}_2-\text{C} & \text{C-Me} \end{array}$$

#### ● HCl

RN 635717-20-3 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-2-ethoxy-1,7-dihydro-1-(2-phenylethyl)-8-(1-piperazinyl)-, monohydrochloride (9CI) (CA INDEX NAME)

Ph-
$$CH_2$$
- $CH_2$ 
 $CH_2$ - $C=C-Me$ 

### HCl

RN 635717-22-5 CAPLUS

CN Acetic acid, [[7-(2-butynyl)-6,7-dihydro-6-oxo-1-(2-phenylethyl)-8-(1-piperazinyl)-1H-purin-2-yl]thio]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

MeO-C-CH<sub>2</sub>-S
N
N
N
N
N
N
N
$$CH_2$$
-C=C-Me

RN 635717-24-7 CAPLUS

CN Glycine, N-[7-(2-butynyl)-6,7-dihydro-6-oxo-1-(2-phenylethyl)-8-(1piperazinyl)-1H-purin-2-yl]-, ethyl ester, monohydrochloride (9CI) (CA
INDEX NAME)

$$\begin{array}{c|c} O & & & & & \\ \hline \text{EtO-C-CH}_2 - \text{NH} & & & & & \\ \hline \text{Ph-CH}_2 - \text{CH}_2 & & & & \\ \hline \end{array}$$

# ● HCl

RN 635717-25-8 CAPLUS

CN Acetamide, 2-[[7-(2-butynyl)-1,7-dihydro-6-oxo-1-(2-phenylethyl)-8-(1-piperazinyl)-1H-purin-2-yl]amino]-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & & \\ H_2N-C-CH_2-NH & & & & N\\ \hline Ph-CH_2-CH_2 & & & & \\ O & & & CH_2-C \Longrightarrow C-Me \end{array}$$

## HCl

RN 635717-26-9 CAPLUS

CN Glycine, N-[7-(2-butynyl)-6,7-dihydro-6-oxo-1-(2-phenylethyl)-8-(1-piperazinyl)-1H-purin-2-yl]-N-methyl-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

RN 635717-28-1 CAPLUS

CN Acetic acid, [[7-(2-butynyl)-6,7-dihydro-6-oxo-1-(2-phenylethyl)-8-(1-piperazinyl)-1H-purin-2-yl]oxy]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

MeO-C-CH<sub>2</sub>-O
N
N
N
N
N
N
$$CH_2-C$$
 $C-Me$ 

#### ● HCl

RN 635717-30-5 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-2-(2-hydroxyethoxy)-1-(2-phenylethyl)-8-(1-piperazinyl)-, monohydrochloride (9CI) (CA INDEX NAME)

## ● HCl

RN 635717-32-7 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-2-(dimethylamino)-1,7-dihydro-1-(2-phenylethyl)-8-(1-piperazinyl)-, monohydrochloride (9CI) (CA INDEX NAME)

## • HCl

RN 635717-35-0 CAPLUS

CN Benzonitrile, 2-[[7-(2-butynyl)-2-(dimethylamino)-6,7-dihydro-6-oxo-8-(1-piperazinyl)-1H-purin-1-yl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me-}\text{C} & \text{C-}\text{CH}_2 \\ \text{CN} & \text{O} \\ \text{CH}_2 & \text{N} \\ \text{Me}_2 \text{N} & \text{N} \end{array}$$

#### HC1

RN 635717-36-1 CAPLUS

CN Acetic acid, [[7-(2-butynyl)-1-[(2-cyanophenyl)methyl]-6,7-dihydro-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]thio]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

### HCl

RN 635717-37-2 CAPLUS

CN Benzonitrile, 2-[[7-(2-butynyl)-6,7-dihydro-2-methoxy-6-oxo-8-(1-piperazinyl)-1H-purin-1-yl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me-}\text{C} & \text{C-}\text{CH}_2 \\ \hline \text{CN} & \text{O} \\ \text{CH}_2 & \text{N} \\ \hline \text{MeO} & \text{N} \\ \end{array}$$

RN 635717-39-4 CAPLUS
CN Acetic acid, [[7-(2-butynyl)-1-(cyanomethyl)-6,7-dihydro-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]thio]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 635717-41-8 CAPLUS
CN Acetic acid, [[1,7-di-2-butynyl-6,7-dihydro-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]thio]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 635717-43-0 CAPLUS
CN 1H-Purine-2-carbonitrile, 1,7-di-2-butynyl-6,7-dihydro-6-oxo-8-(1-piperazinyl)-, monohydrochloride (9CI) (CA INDEX NAME)

RN 635717-45-2 CAPLUS

CN 6H-Purin-6-one, 1,7-di-2-butynyl-1,7-dihydro-2-methoxy-8-(1-piperazinyl)-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{MeO} & \text{N} & \text{N} & \text{N} \\ \text{Me-C} & \text{C-CH}_2 & \text{N} & \text{N} \\ \end{array}$$

#### HCl

RN 635717-46-3 CAPLUS

CN Acetic acid, [[7-(2-butynyl)-6,7-dihydro-6-oxo-8-(1-piperazinyl)-1-(2-propenyl)-1H-purin-2-yl]thio]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

MeO-C-CH<sub>2</sub>-S
N
N
N
N
N
N
$$H_2$$
C
 $CH_2$ -C
 $CH_2$ -C
 $CH_2$ -C
 $CH_2$ -C
 $CH_2$ -C
 $CH_2$ -C

#### HC1

RN 635717-47-4 CAPLUS

CN 1H-Purine-2-carbonitrile, 7-(2-butynyl)-6,7-dihydro-6-oxo-8-(1-piperazinyl)-1-(2-propenyl)-, monohydrochloride (9CI) (CA INDEX NAME)

RN 635717-48-5 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-2-methoxy-8-(1-piperazinyl)-1-(2-propenyl)-, monohydrochloride (9CI) (CA INDEX NAME)

$$_{
m H_2C}$$
  $_{
m CH_2}$   $_{
m CH_2}$   $_{
m CC}$   $_{
m CH_2}$   $_{
m CC}$   $_{
m CH_2}$   $_{
m CH_2}$ 

### ● HCl

RN 635717-49-6 CAPLUS

CN Acetic acid, [[7-(2-butynyl)-6,7-dihydro-1-(2-methoxyethyl)-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]thio]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

## HCl

RN 635717-50-9 CAPLUS

CN 1H-Purine-2-carbonitrile, 7-(2-butynyl)-6,7-dihydro-1-(2-methoxyethyl)-6-oxo-8-(1-piperazinyl)-, monohydrochloride (9CI) (CA INDEX NAME)

MEO-
$$CH_2$$
- $CH_2$ 
 $CH_2$ - $C=C-Me$ 

### HCl

RN 635717-51-0 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-2-methoxy-1-(2-methoxyethyl)-8-(1-piperazinyl)-, monohydrochloride (9CI) (CA INDEX NAME)

MeO-
$$CH_2$$
- $CH_2$ - $CH_$ 

## HCl

RN 635717-53-2 CAPLUS

CN 6H-Purin-6-one, 1,7-dihydro-1-methyl-7-(phenylmethyl)-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 3

CRN 635717-52-1 CMF C17 H20 N6 O

CM 2

RN 635717-55-4 CAPLUS

CN 6H-Purin-6-one, 1-ethyl-1,7-dihydro-7-(phenylmethyl)-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635717-54-3 CMF C18 H22 N6 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635717-57-6 CAPLUS

CN 1H-Purine-1-acetic acid, 6,7-dihydro-6-oxo-7-(phenylmethyl)-8-(1-piperazinyl)-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635717-56-5 CMF C20 H24 N6 O3

CRN 76-05-1 CMF C2 H F3 O2

RN 635717-59-8 CAPLUS

CN 6H-Purin-6-one, 1,7-dihydro-1-(2-methoxyethyl)-7-(phenylmethyl)-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 3

CRN 635717-58-7 CMF C19 H24 N6 O2

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635717-61-2 CAPLUS

CN 6H-Purin-6-one, 1,7-dihydro-7-(phenylmethyl)-8-(1-piperazinyl)-1-(2-propynyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635717-60-1 CMF C19 H20 N6 O

CRN 76-05-1 CMF C2 H F3 O2

RN 635717-63-4 CAPLUS

CN 1H-Purine-1-acetonitrile, 6,7-dihydro-6-oxo-7-(phenylmethyl)-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635717-62-3 CMF C18 H19 N7 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635717-84-9 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-2-[(3-hydroxypropyl)thio]-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX

NAME)

CM 1

CRN 635717-83-8 CMF C17 H24 N6 O2 S

HO- (CH<sub>2</sub>)<sub>3</sub>-S
N
N
N
CH<sub>2</sub>-C
$$=$$
 C-Me

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635717-86-1 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-2-[(2-hydroxypropyl)thio]-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 635717-85-0 CMF C17 H24 N6 O2 S

. Me-CH-CH<sub>2</sub>-S
N
N
N
N
CH<sub>2</sub>-C
$$=$$
 C-Me

CM 2

RN 635717-90-7 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-2-[(2,3-dihydroxypropyl)thio]-1,7-dihydro-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 635717-89-4 CMF C17 H24 N6 O3 S

$$\begin{array}{c|c} \text{OH} & & & \\ \text{HO-CH}_2-\text{CH-CH}_2-\text{S} & & & \\ \text{N} & & & \\ \text{N} & & & \\ \text{N} & & & \\ \text{O} & & & \\ \text{CH}_2-\text{C} & & \\ \text{C-Me} \end{array}$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635717-93-0 CAPLUS

CN Propanoic acid, 3-[[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]thio]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635717-92-9 CMF C17 H22 N6 O3 S

CRN 76-05-1 CMF C2 H F3 O2

RN 635717-96-3 CAPLUS

CN Propanoic acid, 2-[[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]thio]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635717-95-2 CMF C17 H22 N6 O3 S

$$\begin{array}{c|c} \text{Me} & & & \\ \text{HO}_2\text{C}-\text{CH}-\text{S} & & & \\ \text{N} & & & \\ \text{N} & & & \\ \text{N} & & & \\ \text{O} & & & \\ \text{CH}_2-\text{C} & & \\ \text{C}-\text{Me} \end{array}$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635717-99-6 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-[(1methylpropyl)thio]-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA
INDEX NAME)

CM 1

CRN 635717-98-5 CMF C18 H26 N6 O S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635718-02-4 CAPLUS
CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-2(propylthio)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635718-01-3 CMF C17 H24 N6 O S

CM 2

RN 635718-08-0 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-2-(dodecylthio)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635718-07-9 CMF C26 H42 N6 O S

Me- 
$$(CH_2)_{11}$$
-S

N

N

N

 $CH_2$ -C

 $C$ -Me

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635718-10-4 CAPLUS

CN 6H-Purin-6-one, 2-[(2-aminoethyl)thio]-7-(2-butynyl)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI). (CA INDEX NAME)

CM :

CRN 635718-09-1 CMF C16 H23 N7 O S

CRN 76-05-1 CMF C2 H F3 O2

RN 635718-21-7 CAPLUS

CN L-Cysteine, S-[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635718-20-6 CMF C17 H23 N7 O3 S

Absolute stereochemistry.

$$NH_2$$
 $NH_2$ 
 $NH_2$ 

CM 2

CRN 76-05-1 CMF C2 H F3 O2

CN

RN 635718-23-9 CAPLUS

6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-[(2-methylpropyl)thio]-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635718-22-8 CMF C18 H26 N6 O S

i-BuS N N N N N N N 
$$\sim$$
 CH2-C  $\rightleftharpoons$  C-Me

CRN 76-05-1 CMF C2 H F3 O2

RN 635718-25-1 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-2-[(1,2-dimethylpropyl)thio]-1,7-dihydro-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM I

CRN 635718-24-0 CMF C19 H28 N6 O S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635718-33-1 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-2-[(2-furanylmethyl)thio]-1,7-dihydro-1-

methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635718-32-0 CMF C19 H22 N6 O2 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635718-35-3 CAPLUS

CN Acetamide, 2-[[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]thio]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635718-34-2 CMF C16 H21 N7 O2 S

$$\begin{array}{c|c} O & & & & & \\ H_2N-C-CH_2-S & & & N & & N \\ \hline & N & & & N & & \\ & & N & & & N \\ \hline & & & N & & \\ & & & & CH_2-C \end{array} \begin{array}{c} NH & & & \\ & & & \\ CH_2-C \end{array} \begin{array}{c} C-Me \\ \end{array}$$

CM 2

RN 635718-37-5 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-2-[(2-thienylmethyl)thio]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635718-36-4 CMF C19 H22 N6 O S2

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635718-39-7 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-2-[[1-(2-thienyl)ethyl]thio]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635718-38-6 CMF C20 H24 N6 O S2

$$\begin{array}{c|c} & \text{Me} & & \\ & \text{CH-S} & & \\ & \text{N} & & \\ & \text{N} & & \\ & \text{CH}_2\text{-}\text{C} = \text{C-Me} \end{array}$$

CRN 76-05-1 CMF C2 H F3 O2

RN 635718-59-1 CAPLUS

CN Acetamide, N-[2-[[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]thio]ethyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635718-58-0 CMF C18 H25 N7 O2 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635718-71-7 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-2-(2-propenylthio)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635718-70-6 CMF C17 H22 N6 O S

CRN 76-05-1 CMF C2 H F3 O2

RN 635718-73-9 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-[[3-(methylthio)phenyl]amino]-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635718-72-8 CMF C21 H25 N7 O S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635718-77-3 CAPLUS

CN Propanoic acid, 2-[[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]thio]-2-methyl-, mono(trifluoroacetate) (9CI)

(CA INDEX NAME)

CM 1

CRN 635718-76-2 CMF C18 H24 N6 O3 S

$$\begin{array}{c|c} Me & & & \\ HO_2C-C-S & & N & N \\ \hline Me & & N & N \\ \hline Me & & N & N \\ \hline O & & CH_2-C \end{array}$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635718-79-5 CAPLUS
CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-[methyl(1-methylethyl)amino]-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635718-78-4 CMF C18 H27 N7 O

$$\begin{array}{c|c} \text{Me} & & & \\ \text{i-Pr-N} & & & N \\ \text{Me} & & & N \\ \text{O} & & \text{CH}_2-\text{C} \end{array} \subset \text{Me}$$

CM 2

RN 635719-41-4 CAPLUS

CN 3-Pyridinecarboxamide, 6-[[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]amino]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635719-40-3 CMF C20 H23 N9 O2

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635719-45-8 CAPLUS

CN Benzamide, 2-[[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]amino]-N-(1,1-dimethylethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

. CM 1

CRN 635719-44-7 CMF C25 H32 N8 O2

CRN 76-05-1 CMF C2 H F3 O2

RN 635719-47-0 CAPLUS
CN Benzamide, 2-[[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]amino]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635719-46-9 CMF C21 H24 N8 O2

CM 2

RN 635719-53-8 CAPLUS

CN Benzoic acid, 2-[[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]methylamino]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635719-52-7 CMF C22 H25 N7 O3

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635719-57-2 CAPLUS

CN Benzenesulfonamide, 2-[[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]amino]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635719-56-1 CMF C20 H24 N8 O3 S

CRN 76-05-1 CMF C2 H F3 O2

RN 635719-73-2 CAPLUS

CN 1H-Purine-2-acetonitrile, 7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635719-72-1 CMF C16 H19 N7 O

CM 2

RN 635719-77-6 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-(2-oxopropyl)-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635719-76-5 CMF C17 H22 N6 O2

Me-C-CH<sub>2</sub> N N N N N N N N 
$$\sim$$
 CH<sub>2</sub>-C $\rightleftharpoons$  C-Me

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635719-79-8 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-2-ethynyl-1,7-dihydro-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635719-78-7 CMF C16 H18 N6 O

HC 
$$=$$
 C  $=$  N  $=$  N  $=$  NH  $=$  NH  $=$  CH<sub>2</sub>  $=$  C  $=$  C  $=$  Me

CM 2

RN 635719-81-2 CAPLUS

CM 1

CRN 635719-80-1 CMF C17 H24 N6 O2 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635719-83-4 CAPLUS

CN Acetamide, N-acetyl-N-[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635719-82-3 CMF C18 H23 N7 O3

Ac2N N N N N N 
$$\sim$$
 NH  $\sim$  NH

CRN 76-05-1 CMF C2 H F3 O2

RN 635719-85-6 CAPLUS

CN Acetamide, N-[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635719-84-5 CMF C16 H21 N7 O2

ACNH N N NH

Me 
$$CH_2-C$$
  $C-Me$ 

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635719-87-8 CAPLUS

CN Acetonitrile, [[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]oxy]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 635719-86-7 CMF C16 H19 N7 O2

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635719-89-0 CAPLUS

CN Guanidine, [7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635719-88-9 CMF C15 H21 N9 O

$$\begin{array}{c|c} NH & & & \\ H_2N-C-NH & N & N & N \\ \hline \\ Me & & N & N \\ \hline \\ CH_2-C \Longrightarrow C-Me \\ \end{array}$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635719-91-4 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-2-(methylthio)-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635719-90-3 CMF C14 H18 N6 O S

$$\begin{array}{c|c} \text{MeS} & \text{H} & \text{N} & \text{NH} \\ \hline \text{N} & \text{N} & \text{N} & \text{NH} \\ \hline \text{N} & \text{N} & \text{CH}_2\text{-}\text{C} \end{array} \subset \text{C-Me}$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635719-93-6 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-2-[(1-methylethyl)thio]-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635719-92-5 CMF C16 H22 N6 O S

i-Prs 
$$\stackrel{H}{\underset{N}{\bigvee}}$$
  $\stackrel{N}{\underset{N}{\bigvee}}$   $\stackrel{NH}{\underset{N}{\bigvee}}$   $\stackrel{NH}{\underset{CH_2-C}{\Longrightarrow}}$   $\stackrel{C-Me}{=}$ 

CRN 76-05-1 CMF C2 H F3 O2

RN 635719-95-8 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-2-[(1,1-dimethylethyl)thio]-1,7-dihydro-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635719-94-7 CMF C17 H24 N6 O S

t-Bus 
$$\stackrel{H}{\underset{N}{\bigvee}}$$
  $\stackrel{N}{\underset{N}{\bigvee}}$   $\stackrel{N}{\underset{N}{\bigvee}}$   $\stackrel{N}{\underset{N}{\bigvee}}$   $\stackrel{N}{\underset{N}{\bigvee}}$   $\stackrel{N}{\underset{N}{\bigvee}}$   $\stackrel{N}{\underset{N}{\bigvee}}$   $\stackrel{N}{\underset{N}{\bigvee}}$   $\stackrel{N}{\underset{N}{\bigvee}}$   $\stackrel{N}{\underset{N}{\bigvee}}$   $\stackrel{N}{\underset{N}{\bigvee}}$ 

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635719-97-0 CAPLUS

CN 1H-Purine-2-carbonitrile, 7-(2-butynyl)-6,7-dihydro-6-oxo-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635719-96-9 CMF C14 H15 N7 O

CRN 76-05-1 CMF C2 H F3 O2

RN 635720-02-4 CAPLUS

CN 1H-Purine-2-carbonitrile, 7-(2-butynyl)-1-[(2-cyanophenyl)methyl]-6,7-dihydro-6-oxo-8-(1-piperazinyl)-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me-}\text{C} & \text{C-}\text{CH}_2 \\ \hline \text{CN} & \text{O} \\ \text{CH}_2 & \text{N} & \text{N} \\ \\ \text{NC} & \text{N} & \text{N} \end{array}$$

# • HCl

RN 635720-16-0 CAPLUS

CN 1H-Purine-2-carbonitrile, 7-(2-butynyl)-1-[(4-cyanophenyl)methyl]-6,7-dihydro-6-oxo-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635720-15-9 CMF C22 H20 N8 O

$$\begin{array}{c|c} \text{NC} & \text{C-CH}_2 \\ \text{O} & \text{N} \\ \text{NC} & \text{N} \\ \end{array}$$

CRN 76-05-1 CMF C2 H F3 O2

RN 635720-18-2 CAPLUS

CN Benzonitrile, 4-[[7-(2-butynyl)-6,7-dihydro-2-(methylthio)-6-oxo-8-(1-piperazinyl)-1H-purin-1-yl]methyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635720-17-1 CMF C22 H23 N7 O S

$$\begin{array}{c|c} \text{Me-C} & \text{C-CH}_2 \\ \text{NC} & \text{O} & \text{N} \\ \text{CH}_2 & \text{N} & \text{N} \\ \\ \text{MeS} & \text{N} & \text{N} \end{array}$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635720-22-8 CAPLUS

CN 1H-Purine-2-carbonitrile, 7-(2-butynyl)-1-[(3-cyanophenyl)methyl]-6,7-

dihydro-6-oxo-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635720-21-7 CMF C22 H20 N8 O

$$\begin{array}{c|c} & CH_2-C \Longrightarrow C-Me \\ \hline NC & N & N \\ \hline NC & N & NH \\ \end{array}$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635720-25-1 CAPLUS

CN 1H-Purine-2-carbonitrile, 8-(3-amino-1-piperidinyl)-7-(2-butynyl)-1-[(2-cyanophenyl)methyl]-6,7-dihydro-6-oxo-, monohydrochloride (9CI) (CA INDEX NAME)

$$CH_2$$
 $CH_2$ 
 $CH_2$ 
 $CH_2$ 
 $CH_2$ 
 $CH_2$ 
 $CH_2$ 
 $CH_2$ 
 $CH_2$ 
 $CH_2$ 
 $CH_2$ 

#### HCl

RN 635720-26-2 CAPLUS

CN Benzonitrile, 2-[[8-(3-amino-1-piperidinyl)-7-(2-butynyl)-6,7-dihydro-2-methoxy-6-oxo-1H-purin-1-yl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

# ● HCl

RN 635720-27-3 CAPLUS

CN 1H-Purine-2-carbonitrile, 8-(3-amino-1-piperidiny1)-7-(2-butyny1)-6,7-dihydro-6-oxo-1-(2-phenylethy1)-, monohydrochloride (9CI) (CA INDEX NAME)

# ● HCl

RN 635720-28-4 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-7-(2-butynyl)-1,7-dihydro-2-methoxy-1-(2-phenylethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

### ● HCl

RN 635720-29-5 CAPLUS

CN 1H-Purine-2-carbonitrile, 8-(3-amino-1-piperidinyl)-7-(2-butynyl)-1-[(4-cyanophenyl)methyl]-6,7-dihydro-6-oxo-, monohydrochloride (9CI) (CA INDEX NAME)

#### ● HCl

RN 635720-30-8 CAPLUS

CN Benzonitrile, 4-[[8-(3-amino-1-piperidinyl)-7-(2-butynyl)-6,7-dihydro-2-methoxy-6-oxo-1H-purin-1-yl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

# ● HCl

RN 635720-34-2 CAPLUS

CN 1H-Purine-2-carbonitrile, 8-(3-amino-1-piperidinyl)-7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635720-33-1 CMF C16 H19 N7 O

NC N N N NH2 NH2 
$$CH_2-C$$
 C-Me

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635720-36-4 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-7-(2-butynyl)-2-[(1,1-dimethylethyl)thio]-1,7-dihydro-1-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635720-35-3 CMF C19 H28 N6 O S

t-BuS N N N NH2 NH2 
$$\sim$$
 CH2-C $\sim$  C-Me

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635720-38-6 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-7-(2-butynyl)-1,7-dihydro-2-methoxy-1-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635720-37-5 CMF C16 H22 N6 O2

MeO N N N NH2 NH2 
$$\sim$$
 CH2-C $\Longrightarrow$  C-Me

CRN 76-05-1 CMF C2 H F3 O2

CN

RN 635720-40-0 CAPLUS

6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-7-(2-butynyl)-2-(diethylamino)-1,7-dihydro-1-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635720-39-7 CMF C19 H29 N7 O

$$\begin{array}{c|c} \text{Et}_2 \text{N} & \text{N} & \text{N} \\ \text{N} & \text{N} & \text{N} \\ \text{Me} & \text{O} & \text{CH}_2 - \text{C} \\ \end{array} \begin{array}{c} \text{CH}_2 - \text{C} \\ \text{C} - \text{Me} \end{array}$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635720-43-3 CAPLUS

CN 1H-Purine-2-carbonitrile, 7-(2-butynyl)-6,7-dihydro-1-methyl-8-[3-(methylamino)-1-piperidinyl]-6-oxo-, monohydrochloride (9CI) (CA INDEX NAME)

NC N N N NHMe NHMe 
$$CH_2-C \equiv C-Me$$

# ● HCl

RN 635720-45-5 CAPLUS

CN 1H-Purine-2-carbonitrile, 8-(3-amino-1-pyrrolidinyl)-7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} NC & N & N & NH_2 \\ \hline N & N & NH_2 \\ \hline Me & CH_2-C \end{array} \subset C-Me$$

# HCl

IT 635717-07-6 635723-88-5

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(preparation of purinone derivs. as dipeptidylpeptidase IV inhibitors)

RN 635717-07-6 CAPLUS

CN 1H-Purine-2-carbonitrile, 7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)

RN 635723-88-5 CAPLUS

CN 1H-Purine-2-carbonitrile, 7-(2-butynyl)-1-[(2-cyanophenyl)methyl]-6,7-dihydro-6-oxo-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)

IT 635722-55-3P 635722-62-2P 635722-67-7P 635722-85-9P 635722-93-9P 635723-71-6P

635723-77-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of purinone derivs. as dipeptidylpeptidase IV inhibitors)

RN 635722-55-3 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[2-(aminocarbonyl)-7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-1H-purin-8-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & O \\ \parallel & & & C-OBu-t \\ H_2N-C & & N & N & N \\ Me & & N & N & CH_2-C \longrightarrow C-Me \end{array}$$

RN 635722-62-2 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[7-(2-butynyl)-1-[(2-cyanophenyl)methyl]-2-(dimethylamino)-6,7-dihydro-6-oxo-1H-purin-8-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$CH_2$$
 $CH_2$ 
 $CH_2$ 

RN 635722-67-7 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[6,7-dihydro-6-oxo-7-(phenylmethyl)-1H-purin-8-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 635722-85-9 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[7-(2-butynyl)-2-cyano-1-[(2-cyanophenyl)methyl]-6,7-dihydro-6-oxo-1H-purin-8-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$CH_2$$
 $CH_2$ 
 $CH_2$ 

RN 635722-93-9 CAPLUS

CN Carbamic acid, [1-[7-(2-butynyl)-2-cyano-1-[(2-cyanophenyl)methyl]-6,7-dihydro-6-oxo-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 635723-71-6 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[7-(2-chlorophenyl)-2-(2-ethoxy-2-oxoethoxy)-6,7-dihydro-1-methyl-6-oxo-1H-purin-8-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 635723-77-2 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[7-(2-butynyl)-2-cyano-6,7-dihydro-1-methyl-6-oxo-1H-purin-8-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

NC N N N N CH<sub>2</sub>-C 
$$=$$
 C-Me

REFERENCE COUNT:

THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 2 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN DUPLICATE 2

ACCESSION NUMBER:

1995:863353 CAPLUS

DOCUMENT NUMBER:

123:286062

TITLE:

Polycyclic guanine derivatives as phosphodiesterase

enzyme inhibitors and antihypertensives

INVENTOR(S):

Neustadt, Bernard R.; Lindo, Neil A.; McKittrick,

Brian A.

PATENT ASSIGNEE(S):

Schering Corp., USA

SOURCE:

U.S., 32 pp. Cont.-in-part of U.S. Ser. No. 514, 568,

abandoned.

CODEN: USXXAM

DOCUMENT TYPE:

Patent

LANGUAGE:

ED

GΙ

English

FAMILY ACC. NUM. COUNT:

19 Oct 1995

PATENT INFORMATION:

Entered STN:

PATENT NO.	KIND DATE	APPLICATION NO.	DATE			
US 5393755	A 19950228	US 1992-949811	19921214			
WO 9119717	A1 19911226	WO 1991-US4154	19910620			
W: AU, BB, BG,	BR, CA, CS, FI, HU,	JP, KP, KR, LK,	MC, MG, MW, NO,			
PL, RO, SD,	SU, US					
RW: AT, BE, BF,	BJ, CF, CG, CH, CI,	CM, DE, DK, ES,	FR, GA, GB, GN,			
GR, IT, LU,	ML, MR, NL, SE, SN,	TD, TG				
PRIORITY APPLN. INFO.:		US 1990-541568	B2 19900621			
		WO 1991-US4154	W 19910620			
OTHER SOURCE(S):	MARPAT 123:286062					

R3

II

N R2

AΒ Novel polycyclic guanine derivs. I or II wherein J is oxygen or sulfur, R1 is hydrogen, alkyl or alkyl substituted with aryl or hydroxy; R2 is hydrogen, aryl, heteroaryl, cycloalkyl, alkyl or alkyl substituted with aryl, heteroaryl, hydroxy, alkoxy, amino, monoalkyl amino or dialkylamino, or (CH2)mTCOR20 wherein m is an integer from 1 to 6, T is oxygen or NH and R20 is hydrogen, aryl, heteroaryl, alkyl or alkyl substituted with aryl or heteroaryl; R3 is hydrogen, halo, trifluoromethyl, alkoxy, alkylthio, alkyl, cycloalkyl, aryl, aminosulfonyl, amino, monoalkylamino, dialkylamino, hydroxyalkylamino, aminoalkylamino, carboxy, alkoxycarbonyl

or aminocarbonyl or alkyl substituted with aryl, hydroxy, alkoxy, amino, monoalkylamino or dialkylamino; Ra, Rb, Rc and Rd independently represent hydrogen, alkyl, cycloalkyl or aryl; or (Ra and Rb) or (Rc and Rd) or (Rb and Rc) can complete a saturated ring of 5- to 7-carbon atoms, or (Ra and Rb) taken together and (Rb and Rc) taken together, each complete a saturated ring of 5- to 7-carbon atoms, wherein each ring optionally can contain a sulfur or oxygen atom and whose carbon atoms may be optionally substituted with one or more or the following: alkenyl, alkynyl, hydroxy, carboxy, alkoxycarbonyl, alkyl or alkyl substituted with hydroxy, carboxy or alkoxycarbonyl; or such saturated ring can have two adjacent carbon atoms which are shared with an adjoining aryl ring; and n is zero or one. The compds. of formulas (I) and (II) are useful as antihypertensive, muscle relaxant and bronchodilating agents. Thus, e.g., imidazopurinone III, prepared by cyclization of 2-(trans-2-hydroxycyclopentylamino)-1-methyl-7-(phenylmethyl)purin-6-one (preparation given) with SOCl2, inhibited phosphodiesterase enzymes calcium-calmodulin dependent phosphodiesterase (CaM-PDE) and cGMP phosphodiesterase (cGMP-PDE) with IC50 values of 0.3 and 0.4 µM, resp. In vivo antihypertensive activity of III was determined orally in spontaneously hypertensive rats: at 25 mpk dose, fall in mean blood pressure of 30 mm Hq was observed Pharmaceutical formulations were

IT 140396-39-0P, 2-(trans-2-Hydroxycyclopentylamino)-1-methyl-8phenyl-7-(phenylmethyl)purin-6-one 140396-40-3P,

2-(trans-2-Hydroxycyclohexylamino)-1-methyl-8-phenyl-7-(phenylmethyl)purin-

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(polycyclic guanine derivs. as phosphodiesterase enzyme inhibitors and antihypertensives)

RN 140396-39-0 CAPLUS

CN 6H-Purin-6-one, 1,7-dihydro-2-[(2-hydroxycyclopentyl)amino]-1-methyl-8-phenyl-7-(phenylmethyl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 140396-40-3 CAPLUS

CN 6H-Purin-6-one, 1,7-dihydro-2-[(2-hydroxycyclohexyl)amino]-1-methyl-8-phenyl-7-(phenylmethyl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L32 ANSWER 3 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN DUPLICATE 3

ACCESSION NUMBER: 1992:448192 CAPLUS

DOCUMENT NUMBER: 117:48192

TITLE: Studies on purines - part I: Preparation and

antimicrobial activity of 2-amino-4-hydroxy-8-(2'-aryl-

6'/7'-substituted quinolin-4'-yl)purines and their

Mannich bases

AUTHOR(S): Lakhani, R. R.; Parikh, A. R.

CORPORATE SOURCE: Dep. Chem., Saurashtra Univ., Rajkot, 360005, India SOURCE: Acta Ciencia Indica, Chemistry (1991), 17C(1), 47-54

CODEN: ACICDV; ISSN: 0253-7338

DOCUMENT TYPE: Journal LANGUAGE: English ED Entered STN: 08 Aug 1992

GI

The title compds. I (R = HO, MeO, R1, R2 = H, MeO, Me, O2N, C1) were ΑB prepared by cyclocondensation of quinolinecarboxylic acids with 2,4,5-triamino-6-hydroxypyrimidine followed by Mannich reaction with The prepared compds. were tested for bactericidal activity.

141853-43-2P 141853-44-3P 141853-45-4P 141853-46-5P 141853-47-6P 141853-48-7P 141853-49-8P 141853-50-1P 141853-51-2P 141853-52-3P 141853-53-4P 141853-54-5P 141853-55-6P 141853-56-7P 141853-57-8P

141853-58-9P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

141853-43-2 CAPLUS RN

6H-Purin-6-one, 2-amino-7-[(diethylamino)methyl]-1,7-dihydro-8-[2-(4hydroxyphenyl)-7-methoxy-4-quinolinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & &$$

RN 141853-44-3 CAPLUS

CN 6H-Purin-6-one, 2-amino-7-[(diethylamino)methyl]-1,7-dihydro-8-[2-(4-hydroxyphenyl)-6-methoxy-4-quinolinyl]- (9CI) (CA INDEX NAME)

RN 141853-45-4 CAPLUS

CN 6H-Purin-6-one, 2-amino-7-[(diethylamino)methyl]-1,7-dihydro-8-[2-(4-hydroxyphenyl)-7-methyl-4-quinolinyl]- (9CI) (CA INDEX NAME)

RN 141853-46-5 CAPLUS

CN 6H-Purin-6-one, 2-amino-7-[(diethylamino)methyl]-1,7-dihydro-8-[2-(4-hydroxyphenyl)-6-methyl-4-quinolinyl]- (9CI) (CA INDEX NAME)

RN 141853-47-6 CAPLUS

CN 6H-Purin-6-one, 2-amino-7-[(diethylamino)methyl]-1,7-dihydro-8-[2-(4-hydroxyphenyl)-7-nitro-4-quinolinyl]- (9CI) (CA INDEX NAME)

RN 141853-48-7 CAPLUS

CN 6H-Purin-6-one, 2-amino-7-[(diethylamino)methyl]-1,7-dihydro-8-[2-(4-hydroxyphenyl)-6-nitro-4-quinolinyl]- (9CI) (CA INDEX NAME)

RN 141853-49-8 CAPLUS

CN 6H-Purin-6-one, 2-amino-8-[7-chloro-2-(4-hydroxyphenyl)-4-quinolinyl]-7-[(diethylamino)methyl]-1,7-dihydro-(9CI) (CA INDEX NAME)

RN 141853-50-1 CAPLUS

CN 6H-Purin-6-one, 2-amino-8-[6-chloro-2-(4-hydroxyphenyl)-4-quinolinyl]-7-[(diethylamino)methyl]-1,7-dihydro- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ &$$

RN 141853-51-2 CAPLUS

CN 6H-Purin-6-one, 2-amino-7-[(diethylamino)methyl]-1,7-dihydro-8-[7-methoxy-2-(4-methoxyphenyl)-4-quinolinyl]- (9CI) (CA INDEX NAME)

RN 141853-52-3 CAPLUS

CN 6H-Purin-6-one, 2-amino-7-[(diethylamino)methyl]-1,7-dihydro-8-[6-methoxy-2-(4-methoxyphenyl)-4-quinolinyl]- (9CI) (CA INDEX NAME)

RN 141853-53-4 CAPLUS

CN 6H-Purin-6-one, 2-amino-7-[(diethylamino)methyl]-1,7-dihydro-8-[2-(4-methoxyphenyl)-7-methyl-4-quinolinyl]- (9CI) (CA INDEX NAME)

RN 141853-54-5 CAPLUS

CN 6H-Purin-6-one, 2-amino-7-[(diethylamino)methyl]-1,7-dihydro-8-[2-(4-methoxyphenyl)-6-methyl-4-quinolinyl]- (9CI) (CA INDEX NAME)

RN 141853-55-6 CAPLUS

CN 6H-Purin-6-one, 2-amino-7-[(diethylamino)methyl]-1,7-dihydro-8-[2-(4-methoxyphenyl)-7-nitro-4-quinolinyl]- (9CI) (CA INDEX NAME)

RN 141853-56-7 CAPLUS

CN 6H-Purin-6-one, 2-amino-7-[(diethylamino)methyl]-1,7-dihydro-8-[2-(4-methoxyphenyl)-6-nitro-4-quinolinyl]- (9CI) (CA INDEX NAME)

RN 141853-57-8 CAPLUS

CN 6H-Purin-6-one, 2-amino-8-[7-chloro-2-(4-methoxyphenyl)-4-quinolinyl]-7-[(diethylamino)methyl]-1,7-dihydro- (9CI) (CA INDEX NAME)

RN 141853-58-9 CAPLUS

CN 6H-Purin-6-one, 2-amino-8-[6-chloro-2-(4-methoxyphenyl)-4-quinolinyl]-7-[(diethylamino)methyl]-1,7-dihydro-(9CI) (CA INDEX NAME)

L32 ANSWER 4 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN DUPLICATE 4

ACCESSION NUMBER:

1991:608009 CAPLUS

DOCUMENT NUMBER:

115:208009

TITLE:

Preparation of 2-aminopyrimidinones as antihistaminics

and antiserotoninergics

INVENTOR (S):

Janssens, Frans E.; Kennis, Ludo E. J.; Sommen,

Francois M.; Dierckx, Ann C. J.

PATENT ASSIGNEE(S):

Janssen Pharmaceutica N. V., Belg.

SOURCE:

Eur. Pat. Appl., 30 pp.

CODEN: EPXXDW

DOCUMENT TYPE: LANGUAGE:

Patent English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.			APPLICATION NO.	
EP 378254			EP 1990-200004	
EP 378254			EF 1990-200004	19900103
EP 378254				
			B, GR, IT, LI, LU, NL	
US 5008268	A		US 1989-456391	
ES 2058749			ES 1990-200004	
	AA	19900709	CA 1990-2007198	19900105
FI 9000084	Α	19900710	FI 1990-84	19900108
·FI 94526	В	19950615		
FI 94526	. C	19950925		
NO 9000070	Α	19900710	NO 1990-70	19900108
NO 172645	В	19930510		4
NO 172645	С	19930818		
AU 9047780	A1	19900712	AU 1990-47780	19900108
AU 622509	B2	19920409	•	
HU 53364	A2	19901028	HU 1990-63	19900108
HU 206350	В	19921028		1,,,,,,,
ZA 9000120	A	19910925	ZA 1990-120	19900108
SU 1825364	A3	19930630		
CN 1044099	A	19900725	CN 1990-100077	19900108
	В		CN 1990-1000//	19900109
			TD 1000 0414	
JP 02233678	A2	19900917		
PRIORITY APPLN. INFO.:			GB 1989-380 A	19890109
OTHER SOURCE(S):	MARPAT	115:208009		

OTHER SOURCE(S):

Entered STN: 15 Nov 1991

The title compds. [I; X1X2X3X4 = (substituted) CH:CHCH:CH, N:CHCH:CH, CH:NCH:CH, CH:CHN:CH, CH:CHCH:N, N:CHN:CH, CH:NCH:N; R1 = H, alkyl, cycloalkyl, arylalkyl, etc.; R2, R3, R6 = H, alkyl; n = 0-2; R4 = H, (substituted) alkyl; R5 = H, alkyl, alkylaminocarbonyl, arylaminocarbonyl; R5R6 = (alkyl-substituted) CH2CH2, CH2CH2CH2, CH:CH, CH:N, N:CH, N:CHCH2; Z = alkylene; Z1 = CH2, O, S, SO, SO2, imino], were prepared Thus, 1-[(4-fluorophenyl)methyl]-2-(4-piperidinylmethyl)-1H-benzimidazole, 4-methyl-2-pentanone, and Na2CO3 were refluxed 42 h to give 51.2% title compound II which had an ED50 of 0.005 mg/kg in rats for reduction of tryptamine-induced hyperemia.

ΙI

IT 131264-36-3P

CN

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as antihistaminic and antiserotoninergic)

RN 131264-36-3 CAPLUS

1,2,4-Triazolo[4,3-a]pyrimidin-5(1H)-one, 6-[2-[4-[[7-[(4-fluorophenyl)methyl]-6,7-dihydro-6-oxo-1H-purin-8-yl]amino]-1-piperidinyl]ethyl]-1,3,7-trimethyl- (9CI) (CA INDEX NAME)

L32 ANSWER 5 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN DUPLICATE 5

ACCESSION NUMBER:

1988:217553 CAPLUS

DOCUMENT NUMBER:

108:217553

TITLE:

Synthesis and identification of benzo[a]pyrene-guanine nucleoside adducts formed by electrochemical oxidation and by horseradish peroxidase catalyzed reaction of

benzo[a]pyrene with DNA

AUTHOR (S):

Rogan, E. G.; Cavalieri, E. L.; Tibbels, S. R.; Cremonesi, P.; Warner, C. D.; Nagel, D. L.; Tomer, K.

B.; Cerny, R. L.; Gross, M. L.

CORPORATE SOURCE:

Dep. Pharm. Sci., Univ. Nebraska Med. Cent., Omaha,

NE, 68105-1065, USA

SOURCE:

Journal of the American Chemical Society (1988),

110(12), 4023-9

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE:

Journal English LANGUAGE:

OTHER SOURCE(S):

CASREACT 108:217553

Entered STN: 24 Jun 1988

GI

The synthesis of adducts by anodic oxidation of benzo[a]pyrene (BP) in the presence of deoxyguanosine (dG) or guanosine (G) is reported. By using 1H and 2-dimensional NMR spectroscopy as well as fast atom bombardment and collisionally activated decomposition (CAD) mass spectrometry, adducts were identified as BP bound at C-6-C-8 of guanine (Gua), dG, and G and to N-7 of Gua. Loss of deoxyribose from the N-7 adduct was anticipated, but it was unexpectedly found that .apprx.30% of the C-8 adduct with dG lost the deoxyribose moiety. The C-8 adduct of G almost entirely retained the ribose moiety. These compds. were used as markers for HPLC to identify adducts formed in the horseradish peroxidase-catalyzed binding of BP to DNA. By use of HPLC in 2 solvent systems, adducts were identified in the supernatant fraction obtained after EtOH precipitation of the DNA and in an enzymic digest of the DNA. The supernatant, containing adducts lost by depurination, afforded 95% of the N-7 adduct and .apprx.50% of the C-8 adduct. The major adduct identified in the DNA digest was the C-8 of dG (I). The structure of the N-7 adduct in the supernatant was confirmed by CAD mass spectrometry. Thus, horseradish peroxidase catalyzes binding of BP to DNA by 1-electron oxidation

IT 114378-33-5

RL: FORM (Formation, nonpreparative)

Ι

(formation of, from benzopyrene under oxidizing conditions)

RN 114378-33-5 CAPLUS

CN 6H-Purin-6-one, 2-amino-7,8-bis(benzo[a]pyren-6-yl)-1,7-dihydro- (9CI) (CA INDEX NAME)

L32 ANSWER 6 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2004:965251 CAPLUS

DOCUMENT NUMBER:

141:410949

TITLE:

Preparation of fused imidazole derivatives as DPP-IV

inhibitors

INVENTOR(S):

Nakahira, Hiroyuki; Hochigai, Hitoshi

PATENT ASSIGNEE(S):

Sumitomo Pharmaceuticals Co., Ltd., Japan PCT Int. Appl., 335 pp.

SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

FAMILY ACC. NUM. COUNT:

Japanese

PATENT INFORMATION:

PAT	CENT	NO.			KIN	)	DATE		i	APPL:	ICAT:	ION 1	NO.		D	ATE		
WO	2004	0968	06		A1	-	2004	1111	1	WO 2	004-	JP61	04		20	00404	127	
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	ΒZ,	CA,	CH,	
		CN,	co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,	
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,	
		NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	
		ТJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	zw	
	RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	
		AZ,	BY,	KG,	KZ,	MD,	RU,	TJ,	TM,	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	
		EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	IT,	LU,	MC,	NL,	PL,	PT,	RO,	SE,	
·		SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	
		SN,	TD,	TG														
ORITY	APP	LN.	INFO	. :						JP 20	003-	1257	15	1	A 20	00304	130	
									,	JP 20	003-	3524	23	7	A 20	0031	010	

PRIO

OTHER SOURCE(S): MARPAT 141:410949

Entered STN: 12 Nov 2004 ED

GI

$$R^{1}$$
 $N$ 
 $N$ 
 $Y-NH_{2}$ 
 $I$ 

$$Q^1 = -N \qquad \qquad \begin{array}{c} R^4 \\ NH_2 \end{array}$$

The compds. I [R1 represents hydrogen, optionally substituted alkyl, etc.; R2 represents hydrogen, optionally substituted alkyl, optionally substituted aryl, etc.; R3 represents hydrogen, optionally substituted aryl, etc.; and -Y-NH2 represents, e.g., a group represented by Q1 (A is (CH2)m; m is 0, 1, or 2; and R4 is absent, or one or two R4's are present, the R4's each independently representing optionally substituted alkyl, etc.).] are prepared Reaction of 1-methyl-2-dimethylamino-8-bromo-7-benzyl-1,7-dihydro-6H-purin-6-one with (R)-3-aminopiperidine 2HCl salt in ethanol containing diisopropylethylamine at 110°C for 100 h gave, after workup, 2-dimethylamino-8-[(3R)-3-aminopiperidin-1-yl]-7-benzyl-1-methyl-1,7-dihydro-6H-purin-6-one. Compds. of this invention in vitro showed IC50 values of 2 nM to 104 nM against human DPP-IV (dipeptidyl peptidase IV).

TT 791074-69-6P 791074-71-0P 791074-73-2P 791074-75-4P 791074-77-6P 791074-78-7P 791074-79-8P 791074-80-1P 791074-82-3P 791074-85-6P 791074-87-8P 791074-89-0P 791074-91-4P 791074-92-5P 791074-94-7P 791076-43-2P 791076-41-0P 791076-42-1P 791076-48-7P 791076-49-8P 791076-50-1P 791077-07-1P 791077-08-2P 791077-25-3P 791077-26-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of fused imidazole derivs. as DPP-IV inhibitors) 791074-69-6 CAPLUS

CN 6H-Purin-6-one, 8-[(3R)-3-amino-1-piperidinyl]-7-[(2-bromophenyl)methyl]-1,7-dihydro-1-methyl-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN

RN 791074-71-0 CAPLUS

CN Benzonitrile, 2-[[8-[(3R)-3-amino-1-piperidinyl]-1,6-dihydro-1-methyl-6-oxo-2-(trifluoromethyl)-7H-purin-7-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 791074-73-2 CAPLUS

CN 6H-Purin-6-one, 8-[(3R)-3-amino-1-piperidinyl]-7-[(2-bromophenyl)methyl]-1,7-dihydro-2-methyl-1-(2-oxo-2-phenylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 791074-75-4 CAPLUS

CN 6H-Purin-6-one, 8-[(3R)-3-amino-1-piperidinyl]-7-[(2-bromophenyl)methyl]-1,7-dihydro-1,2-dimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 791074-77-6 CAPLUS

CN 6H-Purin-6-one, 8-[(3R)-3-amino-1-piperidinyl]-7-[(2-bromophenyl)methyl]-1,7-dihydro-1-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 791074-78-7 CAPLUS

CN 6H-Purin-6-one, 8-[(3R)-3-amino-1-piperidinyl]-7-[(2-chlorophenyl)methyl]-1,7-dihydro-1-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 791074-79-8 CAPLUS
CN 6H-Purin-6-one, 8-[(3R)-3-amino-1-piperidinyl]-7-[(2-bromophenyl)methyl]1,7-dihydro-1-(2-oxo-2-phenylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 791074-80-1 CAPLUS
CN 6H-Purin-6-one, 8-[[(1R,2S)-2-aminocyclohexyl]amino]-7-[(2-bromophenyl)methyl]-1,7-dihydro-1-(2-oxo-2-phenylethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 791074-82-3 CAPLUS CN 6H-Purin-6-one, 8-[[(1R,2S)-2-aminocyclohexyl]amino]-7-[(2-

Relative stereochemistry.

RN 791074-85-6 CAPLUS
CN 6H-Purin-6-one, 8-[(3R)-3-amino-1-piperidinyl]-7-[(5-fluoro-2-methylphenyl)methyl]-1,7-dihydro-1-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

bromophenyl)methyl]-1,7-dihydro-1-methyl-, rel- (9CI) (CA INDEX NAME)

CM 1

CRN 791074-84-5 CMF C19 H23 F N6 O

Absolute stereochemistry.

CRN 76-05-1 CMF C2 H F3 O2

RN 791074-87-8 CAPLUS

CN 6H-Purin-6-one, 2-amino-8-(3-amino-1-piperidinyl)-1,7-dihydro-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 791074-89-0 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-2-ethoxy-1,7-dihydro-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 791074-91-4 CAPLUS

CN 6H-Purin-6-one, 8-[(3R)-3-amino-1-piperidinyl]-2-(dimethylamino)-1,7-dihydro-1-methyl-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 791074-92-5 CAPLUS

CN 6H-Purin-6-one, 8-[(3R)-3-amino-1-piperidinyl]-7-[(2-chlorophenyl)methyl]-2-(dimethylamino)-1,7-dihydro-1-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 791074-94-7 CAPLUS

CN 6H-Purin-6-one, 2-amino-8-[(3R)-3-amino-1-piperidinyl]-7-[(2-chlorophenyl)methyl]-1,7-dihydro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 791074-97-0 CAPLUS

CN 6H-Purin-6-one, 8-[(3R)-3-amino-1-piperidinyl]-7-[(2-chlorophenyl)methyl]-1,7-dihydro-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 791076-41-0 CAPLUS

CN 1H-Purine-2-carboxylic acid, 8-[(3R)-3-amino-1-piperidinyl]-7-[(2-chlorophenyl)methyl]-6,7-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 791076-42-1 CAPLUS

CN 1H-Purine-1-acetamide, 8-[(3R)-3-amino-1-piperidinyl]-7-[(2-chlorophenyl)methyl]-2-cyano-6,7-dihydro-6-oxo-N-2-pyridinyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 791076-43-2 CAPLUS

CN 1H-Purine-1-acetic acid, 2-(aminocarbonyl)-8-[(3R)-3-amino-1-piperidinyl]-7-[(2-chlorophenyl)methyl]-6,7-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 791076-44-3 CAPLUS

CN 6H-Purin-6-one, 8-[(3R)-3-amino-1-piperidinyl]-2-benzoyl-7-[(2-chlorophenyl)methyl]-1,7-dihydro-1-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 791076-47-6 CAPLUS

CN 1H-Purine-2-carbonitrile, 8-[(3R)-3-amino-1-piperidinyl]-7-[(2-chlorophenyl)methyl]-6,7-dihydro-1-methyl-6-oxo- (9CI) (CA INDEX NAME)

RN 791076-48-7 CAPLUS

CN 6H-Purin-6-one, 2-acetyl-8-[(3R)-3-amino-1-piperidinyl]-7-[(2-chlorophenyl)methyl]-1,7-dihydro-1-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 791076-49-8 CAPLUS

CN 6H-Purin-6-one, 8-[(3R)-3-amino-1-piperidinyl]-7-[(2-chlorophenyl)methyl]-1,7-dihydro-1-methyl-2-(methylthio)- (9CI) (CA INDEX NAME)

RN 791076-50-1 CAPLUS

CN 6H-Purin-6-one, 8-[(3R)-3-amino-1-piperidinyl]-7-[(2-chlorophenyl)methyl]-1,7-dihydro-1-methyl-2-(methylsulfonyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 791077-07-1 CAPLUS

CN 6H-Purin-6-one, 8-[(3R)-3-amino-1-piperidinyl]-7-[(2-chlorophenyl)methyl]1,7-dihydro-1-methyl-2-(phenylamino)-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 791077-08-2 CAPLUS
CN 6H-Purin-6-one, 8-[(3R)-3-amino-1-piperidinyl]-7-[(2-chlorophenyl)methyl]1,7-dihydro-1-methyl-2-(phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 791077-25-3 CAPLUS
CN 1H-Purine-2-carboxylic acid, 8-[(3R)-3-amino-1-piperidinyl]-7-[(2-chlorophenyl)methyl]-6,7-dihydro-6-oxo-, methyl ester (9CI) (CA INDEX NAME)

RN 791077-26-4 CAPLUS

CN 1H-Purine-2-carboxylic acid, 8-[(3R)-3-amino-1-piperidinyl]-7-[(2-chlorophenyl)methyl]-6,7-dihydro-6-oxo-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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IT
     791075-05-3P 791075-07-5P 791075-92-8P
     791075-93-9P 791075-94-0P 791075-95-1P
     791075-98-4P 791075-99-5P 791076-00-1P
     791076-01-2P 791076-02-3P 791076-03-4P
     791076-04-5P 791076-05-6P 791076-10-3P
     791076-13-6P 791076-14-7P 791076-15-8P
     791076-16-9P 791076-19-2P 791076-20-5P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of fused imidazole derivs. as DPP-IV inhibitors)
RN
     791075-05-3 CAPLUS
CN
     Carbamic acid, [(3R)-1-[7-[(2-bromophenyl)methyl]-6,7-dihydro-1-methyl-6-
     oxo-2-(trifluoromethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl
     ester (9CI)
                 (CA INDEX NAME)
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RN 791075-07-5 CAPLUS

CN Carbamic acid, [(3R)-1-[7-[(2-bromophenyl)methyl]-6,7-dihydro-1,2-dimethyl-6-oxo-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 791075-92-8 CAPLUS

CN 1H-Purine-2-carboxylic acid, 7-[(2-chlorophenyl)methyl]-8-[(3R)-3-[[(1,1-dimethylethoxy)carbonyl]amino]-1-piperidinyl]-6,7-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 791075-93-9 CAPLUS

CN Carbamic acid, [(3R)-1-[7-[(2-chlorophenyl)methyl]-2-cyano-6,7-dihydro-6-oxo-1-[2-oxo-2-(2-pyridinylamino)ethyl]-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 791075-94-0 CAPLUS

CN 1H-Purine-1-acetic acid, 7-[(2-chlorophenyl)methyl]-2-cyano-8-[(3R)-3-[[(1,1-dimethylethoxy)carbonyl]amino]-1-piperidinyl]-6,7-dihydro-6-oxo-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 791075-95-1 CAPLUS

CN Carbamic acid, [(3R)-1-[2-benzoyl-7-[(2-chlorophenyl)methyl]-6,7-dihydro-1-methyl-6-oxo-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 791075-98-4 CAPLUS

CN Carbamic acid, [(3R)-1-[7-[(2-chlorophenyl)methyl]-2-cyano-6,7-dihydro-1-methyl-6-oxo-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 791075-99-5 CAPLUS

CN Carbamic acid, [(3R)-1-[2-acetyl-7-[(2-chlorophenyl)methyl]-6,7-dihydro-1-methyl-6-oxo-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 791076-00-1 CAPLUS

CN Carbamic acid, [(3R)-1-[7-[(2-chlorophenyl)methyl]-6,7-dihydro-1-methyl-2-(methylthio)-6-oxo-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 791076-01-2 CAPLUS

CN Carbamic acid, [(3R)-1-[6,7-dihydro-1-methyl-7-[(2-methylphenyl)methyl]-2-(methylthio)-6-oxo-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 791076-02-3 CAPLUS

CN Carbamic acid, [(3R)-1-[7-[(2-chloro-5-fluorophenyl)methyl]-6,7-dihydro-1-methyl-2-(methylthio)-6-oxo-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 791076-03-4 CAPLUS

CN Carbamic acid, [(3R)-1-[7-[(2-chlorophenyl)methyl]-6,7-dihydro-1-methyl-2-(methylsulfonyl)-6-oxo-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 791076-04-5 CAPLUS

CN Carbamic acid, [(3R)-1-[6,7-dihydro-1-methyl-7-[(2-methylphenyl)methyl]-2-(methylsulfonyl)-6-oxo-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 791076-05-6 CAPLUS

CN Carbamic acid, [(3R)-1-[7-[(2-chloro-5-fluorophenyl)methyl]-6,7-dihydro-1-methyl-2-(methylsulfonyl)-6-oxo-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 791076-10-3 CAPLUS

CN Carbamic acid, [(3R)-1-[7-[(2-chlorophenyl)methyl]-6,7-dihydro-1-methyl-6-oxo-2-(phenylamino)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 791076-13-6 CAPLUS

CN 1H-Purine-1-acetic acid, 7-[(2-chlorophenyl)methyl]-8-[(3R)-3-[[(1,1-dimethylethoxy)carbonyl]amino]-1-piperidinyl]-6,7-dihydro-2-(methylsulfonyl)-6-oxo-, 2-propenyl ester (9CI) (CA INDEX NAME)

$$H_2C$$

RN 791076-14-7 CAPLUS

CN 1H-Purine-1-acetic acid, 7-[(2-chlorophenyl)methyl]-8-[(3R)-3-[[(1,1-dimethylethoxy)carbonyl]amino]-1-piperidinyl]-6,7-dihydro-2-(methylthio)-6-oxo-, 2-propenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 791076-15-8 CAPLUS

CN 1H-Purine-1-acetic acid, 7-[(2-chlorophenyl)methyl]-8-[(3R)-3-[[(1,1-dimethylethoxy)carbonyl]amino]-1-piperidinyl]-6,7-dihydro-2-(methylthio)-6-oxo-(9CI) (CA INDEX NAME)

RN 791076-16-9 CAPLUS

CN 1H-Purine-1-acetic acid, 7-[(2-chlorophenyl)methyl]-8-[(3R)-3-[[(1,1-dimethylethoxy)carbonyl]amino]-1-piperidinyl]-6,7-dihydro-2-(methylthio)-6-oxo-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 791076-19-2 CAPLUS

CN 1H-Purine-2-carboxylic acid, 7-[(2-chlorophenyl)methyl]-8-[(3R)-3-[[(1,1-dimethylethoxy)carbonyl]amino]-1-piperidinyl]-6,7-dihydro-6-oxo-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 791076-20-5 CAPLUS

CN 1H-Purine-1-acetic acid, 7-[(2-chlorophenyl)methyl]-2-cyano-8-[(3R)-3-[[(1,1-dimethylethoxy)carbonyl]amino]-1-piperidinyl]-6,7-dihydro-6-oxo-, 2-propenyl ester (9CI) (CA INDEX NAME)

Berch 10/634047

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REFERENCE COUNT:

10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 7 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:287778 CAPLUS

DOCUMENT NUMBER: 140:303701

TITLE: Preparation of piperazine derivatives as dipeptidyl

peptidase IV inhibitors

INVENTOR(S): Yasuda, Nobuyuki; Yamazaki, Kazuto

PATENT ASSIGNEE(S): Eisai Co., Ltd., Japan SOURCE: PCT Int. Appl., 302 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.				KIND		DATE		APPLICATION NO.					DATE				
						-									-		
WO :	WO 2004028524			A1	1 20040408			WO 2003-JP12075					20030922				
	W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	AZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,
		CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	ΕĖ,	EG,	ES,	FI,	GB,	GD,	GE,
		GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KR,	KΖ,	LC,	LK,	LR,
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,	ΝZ,	OM,
		PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	TJ,	TM,	TN,
		TR,	TT,	TZ,	UΑ,	UG,	US,	UΖ,	VC,	VN,	YU,	ZA,	ZM,	zw			
	RW:	GH,	GM,	ΚE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	ŪĠ,	ZM,	ZW,	AM,	ΑZ,	BY,
		KG,	ΚZ,	MD,	RU,	ΤJ,	TM,	AT,	ΒE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,
		FI,	FR,	GB,	GR,	ΗU,	ΙE,	ΙT,	LU,	MC,	ΝL,	PT,	RO,	SE,	SI,	SK,	TR,
		BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG
PRIORITY	PRIORITY APPLN. INFO.:								JP 2002-280137				7	A 20020926			
	JP 2003-117927 A 2003							0030	423								

OTHER SOURCE(S): MARPAT 140:303701

ED Entered STN: 08 Apr 2004

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The title compds. I and II [wherein ring T = (un) substituted heterocyclyl; AB X = (un) substituted alkyl, alkenyl, alkynyl, aryl, heteroaryl, arylalkyl, or heteroarylalkyl; Z1 and Z2 = independently N or (un) substituted CH; R1 and R2 = independently H, (un)substituted alkyl, etc.] or salts or hydrates thereof are prepared as dipeptidyl peptidase (DPP) IV inhibitors in combination with biguanide. For example, the compound III. HCl was prepared in a multi-step synthesis. III-HCl showed inhibitory activity with IC50 of 0.472 nM against DPP IV in pig. I are useful for the treatment of diabetes, obesity, hyperlipidemia, gastrointestinal disturbance, etc. IT 635715-41-2P 635715-48-9P 635715-58-1P 635715-62-7P 635715-63-8P 635715-64-9P 635715-66-1P 635715-81-0P 635715-95-6P 635716-19-7P 635716-65-3P 635716-73-3P 635716-90-4P 635717-00-9P 635717-07-6P

635715-62-7P 635715-63-8P 635715-64-9P 635715-66-1P 635715-81-0P 635715-95-6P 635716-19-7P 635716-65-3P 635716-73-3P 635716-90-4P 635717-00-9P 635717-07-6P 635717-08-7P 635717-10-1P 635717-18-9P 635717-22-5P 635717-35-0P 635717-37-2P 635717-53-2P 635717-93-0P 635718-02-4P 635718-39-7P 635720-02-4P 635720-25-1P 635720-26-2P 635723-88-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of piperazine derivs. as dipeptidyl peptidase IV inhibitors)

RN 635715-41-2 CAPLUS

CN Acetic acid, [[7-(2-chlorophenyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]oxy]-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-40-1 CMF C20 H23 Cl N6 O4

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635715-48-9 CAPLUS

CN Benzeneacetic acid,  $\alpha$ -[[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]oxy]-, methyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-47-8 CMF C23 H26 N6 O4

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635715-58-1 CAPLUS

CN Propanoic acid, 2-[[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]oxy]-, ethyl ester (9CI) (CA INDEX NAME)

RN 635715-62-7 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-2-methoxy-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-61-6 CMF C15 H20 N6 O2

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635715-63-8 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-2-ethoxy-1,7-dihydro-1-methyl-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)

RN 635715-64-9 CAPLUS
CN Acetic acid, [[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]oxy]-, ethyl ester (9CI) (CA INDEX NAME)

Eto-C-CH<sub>2</sub>-O N N N N N N N N  $\sim$  CH<sub>2</sub>-C  $\sim$  C-Me

RN 635715-66-1 CAPLUS

CN Acetic acid, [[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]oxy]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-65-0 CMF C16 H20 N6 O4

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635715-81-0 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1,2-dimethyl-8-(1-piperazinyl)-,

mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-80-9 CMF C15 H20 N6 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635715-95-6 . CAPLUS

6H-Purin-6-one, 7-(2-butynyl)-2-(dimethylamino)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-94-5 CMF C16 H23 N7 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN635716-19-7 CAPLUS

CN6H-Purin-6-one, 7-(2-butynyl)-2-[(2-ethoxyethyl)amino]-1,7-dihydro-1methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM

CRN 635716-18-6 CMF C18 H27 N7 O2

CM2

CRN 76-05-1 CMF C2 H F3 O2

RN635716-65-3 CAPLUS

Alanine, N-[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1Hpurin-2-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM1

CRN 635716-64-2 CMF C17 H23 N7 O3

CM 2

CRN 76-05-1 CMF. C2 H F3 O2

RN 635716-73-3 CAPLUS

CN Acetic acid, [[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]thio]-, methyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-72-2 CMF C17 H22 N6 O3 S

MeO-C-CH<sub>2</sub>-S
N
N
N
N
CH<sub>2</sub>-C
$$\equiv$$
 C-Me

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-90-4 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-[(1-methylethyl)thio]-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-89-1 . CMF C17 H24 N6 O S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635717-00-9 CAPLUS

CN Acetic acid, [[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]thio]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-99-3 CMF C16 H20 N6 O3 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635717-07-6 CAPLUS

CN 1H-Purine-2-carbonitrile, 7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)

RN 635717-08-7 CAPLUS

CN 1H-Purine-2-carbonitrile, 7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635717-07-6 CMF C15 H17 N7 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635717-10-1 CAPLUS

CN 1H-Purine-2-carboxamide, 7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)

RN 635717-18-9 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-2-methoxy-1-(2-phenylethyl)-8-(1-

piperazinyl) -, monohydrochloride (9CI) (CA INDEX NAME)

#### ● HCl

RN 635717-22-5 CAPLUS

CN Acetic acid, [[7-(2-butynyl)-6,7-dihydro-6-oxo-1-(2-phenylethyl)-8-(1-piperazinyl)-1H-purin-2-yl]thio]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

MeO-C-CH<sub>2</sub>-S
N
N
N
N
N
N
N
$$Ph$$
-CH<sub>2</sub>-CH<sub>2</sub>
 $CH_2$ -C
 $CH_2$ -C
 $CH_2$ -C
 $CH_2$ -C
 $CH_2$ -C
 $CH_2$ -C

# HCl

RN 635717-35-0 CAPLUS

CN Benzonitrile, 2-[[7-(2-butynyl)-2-(dimethylamino)-6,7-dihydro-6-oxo-8-(1-piperazinyl)-1H-purin-1-yl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me-}\text{C} & \text{C-}\text{CH}_2 \\ \hline \text{CN} & \text{O} & \\ & \text{CH}_2 & \text{N} & \\ & \text{Me}_2\text{N} & \text{N} & \\ \end{array}$$

## HCl

RN 635717-37-2 CAPLUS

CN Benzonitrile, 2-[[7-(2-butynyl)-6,7-dihydro-2-methoxy-6-oxo-8-(1-piperazinyl)-1H-purin-1-yl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me-}\text{C} & \text{C-}\text{CH}_2 \\ \hline \text{CN} & \text{O} \\ \text{CH}_2 & \text{N} & \text{N} \\ \\ \text{MeO} & \text{N} & \text{N} \end{array}$$

#### ● HCl

RN 635717-53-2 CAPLUS

CN 6H-Purin-6-one, 1,7-dihydro-1-methyl-7-(phenylmethyl)-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635717-52-1 CMF C17 H20 N6 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635717-93-0 CAPLUS

CN Propanoic acid, 3-[[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]thio]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 3

CRN 635717-92-9 CMF C17 H22 N6 O3 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635718-02-4 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-2-(propylthio)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635718-01-3 CMF C17 H24 N6 O S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635718-39-7 CAPLUS

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-2-[[1-(2-thienyl)ethyl]thio]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635718-38-6 CMF C20 H24 N6 O S2

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635720-02-4 CAPLUS

CN 1H-Purine-2-carbonitrile, 7-(2-butynyl)-1-[(2-cyanophenyl)methyl]-6,7-dihydro-6-oxo-8-(1-piperazinyl)-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 635720-25-1 CAPLUS

CN 1H-Purine-2-carbonitrile, 8-(3-amino-1-piperidinyl)-7-(2-butynyl)-1-[(2-cyanophenyl)methyl]-6,7-dihydro-6-oxo-, monohydrochloride (9CI) (CA INDEX NAME)

## • HCl

RN 635720-26-2 CAPLUS

CN Benzonitrile, 2-[[8-(3-amino-1-piperidinyl)-7-(2-butynyl)-6,7-dihydro-2-methoxy-6-oxo-1H-purin-1-yl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

## ● HCl

RN 635723-88-5 CAPLUS

CN 1H-Purine-2-carbonitrile, 7-(2-butynyl)-1-[(2-cyanophenyl)methyl]-6,7-dihydro-6-oxo-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me-C} & \text{C-CH}_2 \\ \hline \text{CN} & \text{O} \\ \hline \text{CH}_2 & \text{N} \\ \hline \text{NC} & \text{N} \\ \end{array}$$

IT 635715-40-1P 635722-55-3P 635722-62-2P

635722-67-7P 635722-85-9P 635722-93-9P

635723-77-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of piperazine derivs. as dipeptidyl peptidase IV inhibitors)

RN 635715-40-1 CAPLUS

CN Acetic acid, [[7-(2-chlorophenyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]oxy]-, ethyl ester (9CI) (CA INDEX NAME)

RN 635722-55-3 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[2-(aminocarbonyl)-7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-1H-purin-8-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & O \\ H_2N-C & N & N & N \\ \hline Me & N & N & N \\ \hline O & CH_2-C \Longrightarrow C-Me \end{array}$$

RN 635722-62-2 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[7-(2-butynyl)-1-[(2-cyanophenyl)methyl]-2-(dimethylamino)-6,7-dihydro-6-oxo-1H-purin-8-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$CH_2$$
 $CH_2$ 
 $CH_2$ 

RN 635722-67-7 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[6,7-dihydro-6-oxo-7-(phenylmethyl)-1H-purin-8-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ H & & & \\ N & & & \\ N & & & \\ N & & & \\ O & & \\ C &$$

RN 635722-85-9 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[7-(2-butynyl)-2-cyano-1-[(2-cyanophenyl)methyl]-6,7-dihydro-6-oxo-1H-purin-8-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 635722-93-9 CAPLUS

CN Carbamic acid, [1-[7-(2-butynyl)-2-cyano-1-[(2-cyanophenyl)methyl]-6,7-dihydro-6-oxo-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 635723-77-2 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[7-(2-butynyl)-2-cyano-6,7-dihydro-1-methyl-6-oxo-1H-purin-8-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

L32 ANSWER 8 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2004:177910 CAPLUS

DOCUMENT NUMBER:

140:235734

TITLE:

Preparation of purine derivatives as

dipeptidylpeptidase IV (DPP-IV) inhibitors.

INVENTOR(S):

Maier, Roland; Himmelsbach, Frank; Eckhardt, Matthias;

US 2002-408021P

P 20020904

Langkopf, Elke; Mark, Michael; Lotz, Ralf

PATENT ASSIGNEE(S):

Boehringer Ingelheim Pharma G.m.b.H. & Co. K.-G.,

Germany

SOURCE:  DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. PATENT INFORMATION	COUNT:	CODEN: Patent German	/ Efen., 38 GWXXBX	Jhi with					
PATENT NO.		KIND	DATE	APPLICAT	ION NO.	D. DATE			
DE 10238477 US 20041222				DE 2002-		20020822 20030804			
WO 20041222	-			WO 2003-					
W: AE,	AG, AL,	AM, AT,	AU, AZ,	BA, BB, BG,	BR, BY,	BZ, CA, CH, CN,			
						GB, GD, GE, GH,			
						KZ, LC, LK, LR,			
						NI, NO, NZ, OM,			
						SY, TJ, TM, TN,			
				VC, VN, YU,					
						ZW, AM, AZ, BY,			
· · · · · · · · · · · · · · · · · · ·						DE, DK, EE, ES,			
						SE, SI, SK, TR,			
		CG, CI,	CM, GA,			NE, SN, TD, TG			
PRIORITY APPLN.	NFO.:			DE 2002-	10238477	A 20020822			

OTHER SOURCE(S):

MARPAT 140:235734

Entered STN: 04 Mar 2004

GI

$$\begin{array}{c|c}
 & 0 \\
 & R^3 \\
 & N \\
 & R^4
\end{array}$$

AB Title compds. [I; R1 = H, (substituted) alkyl, alkenyl, alkynyl, etc.; R2 = H, (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, Ph, heteroaryl, etc.; R3 = (substituted) alkyl, alkenyl, alkynyl, aryl, aralkyl; R4 = substituted azetidin-1-yl, pyrrolidin-1-yl, piperidin-1-yl, hexahydroazepin-1-yl, 3-aminopiperidin-1-yl, etc.], were prepared Thus, [1-(7-benzyl-2-benzylamino-1-methyl-6-oxo-6,7-dihydro-1H-purin-8yl)piperidin-3-yl]carbamic acid tert-Bu ester (preparation given) was stirred 2 h with CF3CO2H in CH2Cl2 to give 73.1% 8-(3-aminopiperidin-1-yl)-7-benzyl-2-benzylamino-1-methyl-1,7-dihydropurin-6-one trifluoroacetate. This inhibited DPP-IV with IC50 = 11 nM. IT 666702-26-7P 666702-31-4P 666702-35-8P 666702-40-5P 666702-45-0P 666702-50-7P 666702-56-3P 666702-63-2P 666702-67-6P 666702-70-1P 666702-73-4P 666702-77-8P 666702-82-5P 666702-86-9P 666702-89-2P 666702-91-6P 666702-94-9P 666702-97-2P 666703-02-2P 666703-05-5P 666703-09-9P 666703-11-3P 666703-14-6P 666703-17-9P 666703-20-4P 666703-21-5P 666703-25-9P 666703-27-1P 666703-29-3P 666703-31-7P 666703-33-9P 666703-35-1P 666703-37-3P 666703-41-9P 666703-45-3P 666703-47-5P 666703-50-0P 666703-52-2P 666703-54-4P 666703-56-6P 666704-19-4P 666704-74-1P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of purine derivs. as dipeptidylpeptidase IV inhibitors) RN666702-26-7 CAPLUS CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-7-

RN 666702-31-4 CAPLUS
CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-2-[[(4-fluorophenyl)methyl]amino]-1,7-dihydro-1-methyl-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

(phenylmethyl) -2-[(phenylmethyl)amino] - (9CI) (CA INDEX NAME)

RN 666702-35-8 CAPLUS CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-2-[(2phenylethyl)amino]-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$Ph-CH_2-CH_2-NH$$
 $N$ 
 $N$ 
 $N$ 
 $NH_2$ 
 $CH_2-Ph$ 

RN 666702-40-5 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-2-[(1-methylethyl)amino]-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 666702-45-0 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-2-(methylamino)-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 666702-50-7 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-2-(cyclohexylamino)-1,7-dihydro-1-methyl-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ NH_{2} & & \\ Me & & \\ &$$

RN 666702-56-3 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-2-[(cyclohexylmethyl)amino]-1,7-dihydro-1-methyl-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 666702-63-2 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-2-(dimethylamino)-1,7-dihydro-1-methyl-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 666702-67-6 CAPLUS

CN 6H-Purin-6-one, 2-amino-8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} H_2N & N & N & N \\ \hline N & N & N & NH_2 \\ \hline Me & CH_2-Ph & \\ \end{array}$$

RN 666702-70-1 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-7-(3-methyl-2-butenyl)-2-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

Ph-CH<sub>2</sub>-NH N NH<sub>2</sub> NH<sub>2</sub> 
$$\sim$$
 CH<sub>2</sub>-CH=CMe<sub>2</sub>

RN 666702-73-4 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1,2-dimethyl-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 666702-77-8 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-7-(3-methyl-2-butenyl)-2-(2-phenylethyl)- (9CI) (CA INDEX NAME)

RN 666702-82-5 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 666702-86-9 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-2-(methylthio)-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 666702-89-2 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-7-(phenylmethyl)-2-[(phenylmethyl)thio]- (9CI) (CA INDEX NAME)

RN 666702-91-6 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-2-(methylthio)-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

MeS N N N NH2 NH2 
$$\sim$$
 CH2-Ph

RN 666702-94-9 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-2-(methylthio)-1-(2-oxo-2-phenylethyl)-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{MeS} & \text{N} & \text{N} \\ \text{O} & \text{N} & \text{N} \\ \text{Ph-C-CH}_2 & \text{O} & \text{CH}_2\text{-Ph} \end{array}$$

RN 666702-97-2 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-2-(methylthio)-1,7-bis(phenylmethyl)- (9CI) (CA INDEX NAME)

MeS N N N NH2
$$Ph-CH_2 O CH_2-Ph$$

RN 666703-02-2 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-2-(methylthio)-1-(2-phenylethyl)-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 666703-05-5 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-(2-oxo-2-phenylethyl)-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & \\ & & \\ \text{Ph-C-CH}_2 & & \\$$

RN 666703-09-9 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-2-[[(4-fluorophenyl)methyl]amino]-1,7-dihydro-1-methyl-7-(phenylmethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 666702-31-4 CMF C25 H28 F N7 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 666703-11-3 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-2-[(2-

phenylethyl)amino]-7-(phenylmethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 666702-35-8 CMF C26 H31 N7 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 666703-14-6 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-2-[(1-methylethyl)amino]-7-(phenylmethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 666702-40-5 CMF C21 H29 N7 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 666703-17-9 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-2-(methylamino)-7-(phenylmethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 666702-45-0 CMF C19 H25 N7 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 666703-20-4 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-2-(cyclohexylamino)-1,7-dihydro-1-methyl-7-(phenylmethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 666702-50-7 CMF C24 H33 N7 O

$$\begin{array}{c|c} & & & \\ & & & \\ NH & & & \\ Me & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 666703-21-5 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-2-[(cyclohexylmethyl)amino]-1,7-dihydro-1-methyl-7-(phenylmethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 666702-56-3 CMF C25 H35 N7 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 666703-25-9 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-2-(dimethylamino)-1,7-dihydro-1-methyl-7-(phenylmethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 666702-63-2 CMF C20 H27 N7 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 666703-27-1 CAPLUS

CN 6H-Purin-6-one, 2-amino-8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-7-(phenylmethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 666702-67-6 CMF C18 H23 N7 O

$$\begin{array}{c|c} H_2N & N & N & N \\ \hline N & N & N & N \\ \hline Me & CH_2-Ph & \\ \end{array}$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 666703-29-3 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-7-(3-methyl-2-butenyl)-2-[(phenylmethyl)amino]-, trifluoroacetate (9CI) (CA INDEX

NAME)

CM 1

CRN 666702-70-1 CMF C23 H31 N7 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

CN

RN 666703-31-7 CAPLUS

6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1,2-dimethyl-7-(phenylmethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 666702-73-4 CMF C19 H24 N6 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 666703-33-9 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-7-(3-methyl-2-butenyl)-2-(2-phenylethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

. -

CRN 666702-77-8

CMF C24 H32 N6 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 666703-35-1 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-7-(phenylmethyl)-, hydrochloride (9CI) (CA INDEX NAME)

•x HCl

RN 666703-37-3 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-2-(methylthio)-7-(phenylmethyl)-, hydrochloride (9CI) (CA INDEX NAME)

•x HCl

RN 666703-41-9 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-2-(methylthio)-1-(2-oxo-2-phenylethyl)-7-(phenylmethyl)-, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{MeS} & \text{N} & \text{N} & \text{N} \\ \text{O} & \text{N} & \text{N} & \text{N} \\ \text{Ph-C-CH}_2 & \text{N} & \text{CH}_2 - \text{Ph} \end{array}$$

•x HCl

RN 666703-45-3 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-2-(methylthio)-1,7-bis(phenylmethyl)-, hydrochloride (9CI) (CA INDEX NAME)

MeS N N N N NH2
$$Ph-CH_{2}$$
 CH2-Ph

•x HCl

RN 666703-47-5 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-2-(methylthio)-1-(2-phenylethyl)-7-(phenylmethyl)-, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{MeS} & \text{N} & \text{N} & \text{N} \\ \text{Ph-CH}_2-\text{CH}_2 & \text{CH}_2-\text{Ph} \end{array}$$

#### •x HCl

RN 666703-50-0 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-7-(phenylmethyl)-2-[(phenylmethyl)thio]-, hydrochloride (9CI) (CA INDEX NAME)

$$Ph-CH_2-S$$
 $N$ 
 $N$ 
 $N$ 
 $NH_2$ 
 $CH_2-Ph$ 

## •x HCl

RN 666703-52-2 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-2-[(2-phenylethyl)thio]-7-(phenylmethyl)-, hydrochloride (9CI) (CA INDEX NAME)

## •x HCl

RN 666703-54-4 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-(2-oxo-2-phenylethyl)-7-(phenylmethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 666703-05-5 CMF C25 H26 N6 O2

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 666703-56-6 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-7-(phenylmethyl)-2-[(phenylmethyl)thio]-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 666702-89-2 CMF C24 H26 N6 O S

$$Ph-CH_2-S$$
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $NH_2$ 
 $CH_2-Ph$ 

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 666704-19-4 CAPLUS

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-7-(phenylmethyl)-2-[(phenylmethyl)amino]-, trifluoroacetate (9CI) (CA INDEX

NAME)

CM 1

CRN 666702-26-7 CMF C25 H29 N7 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

CN

RN 666704-74-1 CAPLUS

6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-2-(methylthio)-7-(phenylmethyl)-, hydrochloride (9CI) (CA INDEX NAME)

MeS N N N N NH2

Me 
$$CH_2-Ph$$

●x HCl

IT 666703-62-4P 666703-64-6P 666703-66-8P 666703-68-0P 666703-78-2P 666703-8P 666703-82-8P 666703-84-0P 666703-86-2P 666703-88-4P 666703-90-8P 666703-92-0P 666703-94-2P 666703-96-4P 666703-98-6P 666704-00-3P 666704-02-5P 666704-04-7P 666704-06-9P 666704-08-1P 666704-09-2P 666704-11-6P 666704-12-7P 666704-13-8P 666704-14-9P 666704-15-0P 666704-16-1P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(preparation of purine derivs. as dipeptidylpeptidase IV inhibitors)

RN 666703-62-4 CAPLUS

CN Carbamic acid, [1-[6,7-dihydro-6-oxo-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
H & N & O \\
N & N & N \\
NH-C-OBu-t
\end{array}$$

$$\begin{array}{c|c}
CH_2-Ph
\end{array}$$

RN 666703-64-6 CAPLUS

CN Carbamic acid, [1-[6,7-dihydro-1-methyl-6-oxo-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} N & N & O \\ \hline N & N & N \\ \hline N & NH-C-OBu-t \\ \hline \\ O & CH_2-Ph \\ \end{array}$$

RN 666703-66-8 CAPLUS

CN Carbamic acid, [1-[6,7-dihydro-6-oxo-1-(2-oxo-2-phenylethyl)-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 666703-68-0 CAPLUS

CN Carbamic acid, [1-[6,7-dihydro-2-(methylthio)-6-oxo-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 666703-74-8 CAPLUS

CN Carbamic acid, [1-[6,7-dihydro-6-oxo-7-(phenylmethyl)-2-[(phenylmethyl)thio]-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 666703-76-0 CAPLUS

CN Carbamic acid, [1-[6,7-dihydro-2-(methylthio)-6-oxo-7-(2-propenyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 666703-78-2 CAPLUS

CN Carbamic acid, [1-[6,7-dihydro-6-oxo-2-[(2-phenylethyl)thio]-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 666703-80-6 CAPLUS

CN Carbamic acid, [1-[6,7-dihydro-1-methyl-2-(methylthio)-6-oxo-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 666703-82-8 CAPLUS

CN Carbamic acid, [1-[6,7-dihydro-2-(methylthio)-6-oxo-1-(2-oxo-2-phenylethyl)-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 666703-84-0 CAPLUS

CN Carbamic acid, [1-[6,7-dihydro-1-methyl-7-(3-methyl-2-butenyl)-2-(methylthio)-6-oxo-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 666703-86-2 CAPLUS

CN Carbamic acid, [1-[6,7-dihydro-2-(methylthio)-6-oxo-1,7-bis(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 666703-88-4 CAPLUS

CN Carbamic acid, [1-[6,7-dihydro-1-methyl-6-oxo-7-(phenylmethyl)-2-[(phenylmethyl)thio]-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 666703-90-8 CAPLUS

CN Carbamic acid, [1-[6,7-dihydro-1-methyl-6-oxo-2-[(2-phenylethyl)thio]-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 666703-92-0 CAPLUS

CN Carbamic acid, [1-[6,7-dihydro-1-methyl-2-(methylsulfinyl)-6-oxo-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Me 
$$\stackrel{\circ}{=}$$
  $\stackrel{\circ}{=}$   $\stackrel$ 

RN 666703-94-2 CAPLUS

CN Carbamic acid, [1-[6,7-dihydro-1-methyl-2-(methylsulfonyl)-6-oxo-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & O & O \\ \hline Me & S & N & N & N \\ \hline O & N & N & N \\ \hline O & NH-C-OBu-t \\ \hline O & CH_2-Ph \\ \end{array}$$

RN 666703-96-4 CAPLUS

CN Carbamic acid, [1-[6,7-dihydro-1-methyl-7-(3-methyl-2-butenyl)-2-(methylsulfinyl)-6-oxo-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Me-S N N N NH-C-OBu-t

Me 
$$\sim$$
 CH<sub>2</sub>-CH= CMe<sub>2</sub>

RN 666703-98-6 CAPLUS

CN Carbamic acid, [1-[6,7-dihydro-1-methyl-6-oxo-7-(phenylmethyl)-2-[(phenylmethyl)amino]-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 666704-00-3 CAPLUS

CN Carbamic acid, [1-[2-[[(4-fluorophenyl)methyl]amino]-6,7-dihydro-1-methyl-6-oxo-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 666704-02-5 CAPLUS

CN Carbamic acid, [1-[6,7-dihydro-1-methyl-6-oxo-2-[(2-phenylethyl)amino]-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 666704-04-7 CAPLUS

CN Carbamic acid, [1-[6,7-dihydro-1-methyl-2-[(1-methylethyl)amino]-6-oxo-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester

#### (9CI) (CA INDEX NAME)

RN 666704-06-9 CAPLUS

CN Carbamic acid, [1-[6,7-dihydro-1-methyl-2-(methylamino)-6-oxo-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 666704-08-1 CAPLUS

CN Carbamic acid, [1-[2-(cyclohexylamino)-6,7-dihydro-1-methyl-6-oxo-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 666704-09-2 CAPLUS

CN Carbamic acid, [1-[2-[(cyclohexylmethyl)amino]-6,7-dihydro-1-methyl-6-oxo-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 666704-11-6 CAPLUS

CN Carbamic acid, [1-[2-(dimethylamino)-6,7-dihydro-1-methyl-6-oxo-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester

(9CI) (CA INDEX NAME)

RN 666704-12-7 CAPLUS

CN Carbamic acid, [1-[2-amino-6,7-dihydro-1-methyl-6-oxo-7-(phenylmethyl)-1Hpurin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX
NAME)

RN 666704-13-8 CAPLUS

CN Carbamic acid, [1-[6,7-dihydro-1-methyl-7-(3-methyl-2-butenyl)-6-oxo-2-[(phenylmethyl)amino]-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 666704-14-9 CAPLUS

CN Carbamic acid, [1-[6,7-dihydro-1,2-dimethyl-6-oxo-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 666704-15-0 CAPLUS

CN Carbamic acid, [1-[6,7-dihydro-1-methyl-7-(3-methyl-2-butenyl)-6-oxo-2-(2-phenylethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI)

### (CA INDEX NAME)

666704-16-1 CAPLUS RN

CN Carbamic acid, [1-[6,7-dihydro-2-(methylthio)-6-oxo-1-(2-phenylethyl)-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

CAPLUS COPYRIGHT 2005 ACS on STN L32 ANSWER 9 OF 17

ACCESSION NUMBER:

1992:651141 CAPLUS

DOCUMENT NUMBER:

117:251141

TITLE:

Preparation of imidazo[2,1-b]purin-4(5H)-ones and

analogs as phosphodiesterase inhibitors

INVENTOR(S):

Neustadt, Bernard R.; Lindo, Neil A.; McKittrick,

Brian A.

PATENT ASSIGNEE(S):

SOURCE:

Schering Corp., USA PCT Int. Appl., 89 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO. K				KIN	D DATE	APPLICATION NO.	DATE	
WO	0 9119717			A1	19911226	WO 1991-US4154	19910620	
	W: AU	, BB,	BG,	BR,	CA, CS, FI,	HU, JP, KP, KR, LK, MC,	MG, MW, NO,	
	$_{ m PL}$	, RO,	SD,	SU,	US			
	RW: AT	, BE,	BF,	вJ,	CF, CG, CH,	CI, CM, DE, DK, ES, FR,	GA, GB, GN,	
	GR	, IT,	LU,	ML,	MR, NL, SE,	SN, TD, TG	•	
ZA	A 9104727			A ·	19920325	ZA 1991-4727	19910619	
CA	2085733			AA	19911222	CA 1991-2085733	19910620	
CA	2085733			С	19960305			
ΑU	9181992			<b>A</b> 1	19920107	AU 1991-81992	19910620	
ΑU	651607			B2	19940728			
ΕP	538332			<b>A</b> 1	19930428	EP 1991-912779	19910620	
ΕP	538332			В1	19970723	•		
	R: AT	, BE,	CH,	DE,	DK, ES, FR,	GB, GR, IT, LI, LU, NL,	SE	
JP	0550864	7		<b>T2</b>	19931202	JP 1991-512084	19910620	
JP	0704758	9		B4	19950524			

HU 65623	A2	19940728	HU 1992-4032	19910620
PL 169481	B1	19960731	PL 1991-297299	19910620
CZ 281920	B6	19970416	CZ 1992-3749	19910620
RU 2080322	C1	19970527	RU 1992-16466	19910620
AT 155786	E	19970815	AT 1991-912779	19910620
US 5393755	Α	19950228	US 1992-949811	19921214
NO 9204940	Α	19921218	NO 1992-4940	19921218
PRIORITY APPLN. INFO.:			US 1990-541568	A2 19900621
			WO 1991-US4154	A 19910620

OTHER SOURCE(S):

MARPAT 117:251141

ED Entered STN: 26 Dec 1992

GI

Title compds. [I; R1 = H, (ar)alkyl, hydroxyalkyl; R2 = H, (cyclo)alkyl, (hetero)aryl, aralkyl, etc.; R3 = H, halo, CF3, alkoxy, (cyclo)alkyl, etc.; R4 - R7 = H, (cyclo)alkyl, aryl; R4R5, R6R7, R5R6 = atoms to complete a ring; X = O, S; n = 0, 1] were prepared Thus, 2-chloro-1-methyl-7-benzylpurin-6-one (preparation given) was condensed with 1-hydroxy-7-aminobicyclo[3.3.0]octane (preparation given) and the product cyclized to give, after optical resolution and deprotection, title compound (+)-II which gave 45 mm Hg reduction in mean blood pressure in rats at 5 mg/kg orally.

IT 140396-39-0P 140396-40-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of phosphodiesterase inhibitors)

RN 140396-39-0 CAPLUS

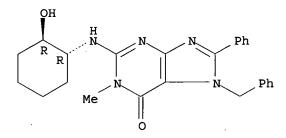
CN 6H-Purin-6-one, 1,7-dihydro-2-[(2-hydroxycyclopentyl)amino]-1-methyl-8-phenyl-7-(phenylmethyl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 140396-40-3 CAPLUS

6H-Purin-6-one, 1,7-dihydro-2-[(2-hydroxycyclohexyl)amino]-1-methyl-8-CN phenyl-7-(phenylmethyl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



CAPLUS COPYRIGHT 2005 ACS on STN L32 ANSWER 10 OF 17

ACCESSION NUMBER: 1989:114567 CAPLUS

DOCUMENT NUMBER: 110:114567

Preparation of (4-Piperidinylmethyl and TITLE:

-hetero) purines as antiallergic agents

(bip 12816 INVENTOR(S): Janssens, Frans Eduard; Diels, Gaston Stanislas

Marcella

PATENT ASSIGNEE(S): Janssen Pharmaceutica N. V., Belg.

SOURCE: Eur. Pat. Appl., 102 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent English LANGUAGE:

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.			APPLICATION NO.		DATE	
EP 206415		19861230	EP 1986-201048	_	19860617	
EP 206415	A3	19880316				
EP 206415	B1	19930127				
R: AT, BE, CH,	DE, FR	, GB, IT,	LI, LU, NL, SE		•	
CA 1267889			CA 1986-511113		19860609	
SU 1581221	A3	19900723	SU 1986-4027617		19860610	
AT 85055	E	19930215	AT 1986-201048		19860617	
JP 62000487		19870106	JP 1986-143155		19860620	
ES 556381	A1	19871116	ES 1986-556381		19860620	
DK 8602952	Α	19861225	DK 1986-2952		19860623	
DK 169073	B1		•			
FI 8602655	Α		FI 1986-2655		19860623	
	В					
FI 85704						
NO 8602504	Α		NO 1986-2504		19860623	
NO 163956	В				•	
NO 163956	С	19900815			•	
AU 8659191	A1	19870108	AU 1986-59191		19860623	
AU 588890	B2	19890928				
HU 42095	A2	19870629	HU 1986-2631		19860623	
HU 199143	В	19900129				
ZA 8604677	Α	19880224			19860623	
/IL 79193		19901105	IL 1986-79193		19860623	
(US 5041448	Α	19910820	US 1989-323250		19890309	
\US 5258380	Α	19931102	US 1991-719273		19910621	
PRIOŘÍTY APPLN. INFO.:			GB 1985-15934	Α	19850624	

US 1986-858339 B1 19860501 EP 1986-201048 A 19860617 US 1989-323250 A3 19890309

Entered STN: 03 Apr 1989 ED GΙ

The title compds. I [A1:A2:A3:A4 = N:CHN:CH, CH:NCH:N, wherein 1 or 2 H AB may each be replaced by halo, C1-6 alkyl, C1-6 alkoxy, F3C, HO; R1 = H, C1-10 alkyl, C3-6 cycloalkyl, etc.; R2 = H, C1-6 alkyl; B = H2C, O, S, SO, SO2, NR, R = H, C1-6 alkyl, C3-6 cycloalkyl, etc.; L = (un) substituted methoxyalkyl, -methylthioalkyl, -alkoxycarbonyl, alkylthio, (un) substituted alkyl, optionally with heteroatom interrupters, (un) substituted N-heterocyclyl, (un) substituted pyrimidinyloxyalkyl, -thioalkyl, etc., with restrictions] and their salts, useful as antiallergic agents, were prepared 2-Ethenylpyridine, 9-[(4fluorophenyl)methyl]-N-(4-piperidinyl)-9H-purin-8-amine and BuOH were refluxed overnight to give 9-[(4-fluorophenyl)methyl]-N-[1-[2-(2pyridinyl)ethyl]-4-piperidinyl]-9H-purin-8-amine (II). In tests in rats against compound 48/80, a potent histamine releasing agent, at 0.5 mg/kg, the ED50 of II was 0.01 mg/kg.

IT 116062-65-8P

> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and alkylation of)

RN116062-65-8 CAPLUS

CN 6H-Purin-6-one, 7-[(4-fluorophenyl)methyl]-1,7-dihydro-8-(4piperidinylamino) -, dihydrobromide (9CI) (CA INDEX NAME)

# •2 HBr

116062-74-9P 116062-92-1P 116063-06-0P IT 116063-46-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as antiallergic agent)

RN116062-74-9 CAPLUS

CN 6H-Purin-6-one, 8-[[1-[(2,3-dihydro-1,4-benzodioxin-2-yl)methyl]-4piperidinyl]amino]-7-[(4-fluorophenyl)methyl]-1,7-dihydro- (9CI) (CA INDEX NAME)

RN 116062-92-1 CAPLUS

CN 6H-Purin-6-one, 7-[(4-fluorophenyl)methyl]-1,7-dihydro-8-[[1-[2-(4-methoxyphenyl)ethyl]-4-piperidinyl]amino]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} H & N & CH_2 - CH_2 \\\hline N & N & CH_2 - CH_2 \\\hline \end{array}$$

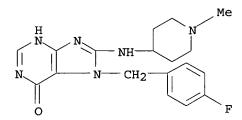
RN 116063-06-0 CAPLUS

CN 4H-Pyrido[1,2-a]pyrimidin-4-one, 3-[2-[4-[[7-[(4-fluorophenyl)methyl]-6,7-dihydro-6-oxo-1H-purin-8-yl]amino]-1-piperidinyl]ethyl]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} H & N & CH_2 - CH_2 \\ \hline N & N - CH_2 \\ \hline \\ O & F \end{array}$$

RN 116063-46-8 CAPLUS

CN 6H-Purin-6-one, 7-[(4-fluorophenyl)methyl]-1,7-dihydro-8-[(1-methyl-4-piperidinyl)amino]- (9CI) (CA INDEX NAME)



L32 ANSWER 11 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1975:85532 CAPLUS

DOCUMENT NUMBER: 82:85532

TITLE: Nuclear magnetic resonance study of hindered rotation

in 8-phenylpurines

AUTHOR(S): Bergmann, F.; Tamir, I.; Neiman, Z.; Lichtenberg, D. CORPORATE SOURCE: Hadassah Med. Sch., Hebrew Univ., Jerusalem, Israel

SOURCE: Haddassan Med. Sch., Hebrew Univ., Jerusalem, Isr

CODEN. TETRAD. TCCN. 0040 4020

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal LANGUAGE: English ED Entered STN: 12 May 1984

AB In the PMR spectrum of 8-phenylpurines, the multiplet of the ortho protons appeared downfield of the multiplet characteristic for meta and para protons. The separation of the centers of these 2 signals diminished with increasing steric interference between the Ph ring and substituents in the imidazole moiety. The contribution of the purine ring current to the chemical shifts of the aromatic protons was calculated by the theory of C. E. Johnson and F. A. Bovey (1958) and the torsion angles between the Ph ring and the plane of the purine system were derived.

IT 32533-56-5 32533-63-4 32533-68-9

RL: PRP (Properties)

(hindered rotation in, PMR in relation to)

RN 32533-56-5 CAPLUS

CN 6H-Purin-6-one, 1,7-dihydro-1,7-dimethyl-8-phenyl- (9CI) (CA INDEX NAME)

RN 32533-63-4 CAPLUS

CN 6H-Purine-6-thione, 1,7-dihydro-1,7-dimethyl-8-phenyl- (9CI) (CA INDEX NAME)

32533-68-9 CAPLUS RN

6H-Purine-6-thione, 1,7-dihydro-7-methyl-8-phenyl- (9CI) (CA INDEX NAME) CN

$$\bigcap_{N} \bigcap_{N} \bigcap_{N} \bigcap_{Me} \bigcap_{Me} \bigcap_{N} \bigcap_{Me} \bigcap_{N} \bigcap_{Me} \bigcap_{N} \bigcap_{Me} \bigcap_{Me} \bigcap_{N} \bigcap_{Me} \bigcap_{N} \bigcap_{Me} \bigcap_{Me} \bigcap_{N} \bigcap_{Me} \bigcap_{Me} \bigcap_{N} \bigcap_{Me} \bigcap_{$$

L32 ANSWER 12 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN

1971:435951 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 75:35951

Methylation of 6-(methylthio)-8-phenylpurines TITLE:

AUTHOR (S): Bergmann, F.; Neiman, Z.; Lichtenberg, D.; Deutsch, J.

Hadassah Med. Sch., Heb. Univ., Jerusalem, Israel CORPORATE SOURCE:

Journal of the Chemical Society [Section] C: Organic SOURCE:

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Methylation of 6-(methylthio)-8-phenylpurine (I) derivs. with MeI-DMF always gave a single product. I and its 7- and 9-Me derivs. were substituted at N-3; the 1-Me derivative was attacked at N-9 and the 3-Me  $\,$ derivative at N-7. The most important difference between the 8-unsubstituted and 8-Ph series was found for the 9-Me derivative Similarly, 9-methyl-8-phenylhypoxanthine was converted into the corresponding 3,9-dimethyl derivative, in contrast to the behavior of the nonphenylated compound

32533-56-5P 32533-63-4P 32533-68-9P IT

> RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

32533-56-5 CAPLUS RN

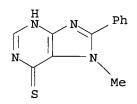
6H-Purin-6-one, 1,7-dihydro-1,7-dimethyl-8-phenyl- (9CI) (CA INDEX NAME) CN

RN 32533-63-4 CAPLUS

6H-Purine-6-thione, 1,7-dihydro-1,7-dimethyl-8-phenyl- (9CI) (CA INDEX CN

RN 32533-68-9 CAPLUS

CN 6H-Purine-6-thione, 1,7-dihydro-7-methyl-8-phenyl- (9CI) (CA INDEX NAME)



L32 ANSWER 13 OF 17 USPATFULL on STN

ACCESSION NUMBER: 2004:159424 USPATFULL

TITLE:

New purine derivatives, the preparation thereof and

their use as pharmaceutical compositions

INVENTOR(S):

Maier, Roland, Biberach, GERMANY, FEDERAL REPUBLIC OF Himmelsbach, Frank, Mittelbiberach, GERMANY, FEDERAL

REPUBLIC OF

Eckhardt, Matthias, Biberach, GERMANY, FEDERAL REPUBLIC

OF

Langkopf, Elke, Warthausen, GERMANY, FEDERAL REPUBLIC

OF

Mark, Michael, Biberach, GERMANY, FEDERAL REPUBLIC OF

Lotz, Ralf R. H., Schemmerhofen, GERMANY, FEDERAL

REPUBLIC OF

PATENT ASSIGNEE(S):

Boehringer Ingelheim Pharma GmbH & Co. KG, Ingelheim,

GERMANY, FEDERAL REPUBLIC OF (non-U.S. corporation)

NUMBER DATE

PRIORITY INFORMATION: DE 2002-10238477 20020822

US 2002-408021P 20020904 (60)

DOCUMENT TYPE: Utility FILE SEGMENT: APPLICATION

LEGAL REPRESENTATIVE: BOEHRINGER INGELHEIM CORPORATION, 900 RIDGEBURY ROAD,

P. O. BOX 368, RIDGEFIELD, CT, 06877

NUMBER OF CLAIMS: 8
EXEMPLARY CLAIM: 1
LINE COUNT: 3088

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The invention relates to new purine derivatives of general formula

##STR1##

wherein R.sup.1 to R.sup.4 are defined as in the claims, the tautomers, the stereoisomers, the mixtures, the prodrugs thereof and the salts thereof, particularly the physiologically acceptable salts thereof with inorganic or organic acids or bases which have valuable pharmacological properties, particularly an inhibiting effect on the activity of the enzyme dipeptidylpeptidase-IV (DPP-IV), the preparation thereof, the use thereof for the prevention or treatment of diseases or conditions associated with an increased DPP-IV activity or capable of being prevented or alleviated by reducing the DPP-IV activity, particularly type I or type II diabetes mellitus, the pharmaceutical compositions containing a compound of general formula (I) or a physiologically acceptable salt thereof as well as processes for the preparation thereof.

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CAS INDEXING IS AVAILABLE FOR THIS PATENT.
   666702-26-7P 666702-31-4P 666702-35-8P
      666702-40-5P 666702-45-0P 666702-50-7P
      666702-56-3P 666702-63-2P 666702-67-6P
      666702-70-1P 666702-73-4P 666702-77-8P
      666702-82-5P 666702-86-9P 666702-89-2P
      666702-91-6P 666702-94-9P 666702-97-2P
      666703-02-2P 666703-05-5P 666703-09-9P
      666703-11-3P 666703-14-6P 666703-17-9P
      666703-20-4P 666703-21-5P 666703-25-9P
      666703-27-1P 666703-29-3P 666703-31-7P
      666703-33-9P 666703-35-1P 666703-37-3P
      666703-41-9P 666703-45-3P 666703-47-5P
      666703-50-0P 666703-52-2P 666703-54-4P
      666703-56-6P 666704-19-4P 666704-74-1P
        (preparation of purine derivs. as dipeptidylpeptidase IV inhibitors)
RN
     666702-26-7 USPATFULL
     6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-7-
CN
       (phenylmethyl) -2-[(phenylmethyl)amino] - (9CI)
                                                     (CA INDEX NAME)
```

RN 666702-35-8 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-2-[(2-phenylethyl)amino]-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$Ph-CH_2-CH_2-NH$$
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $NH_2$ 
 $CH_2-Ph$ 

RN 666702-40-5 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-2-[(1-methylethyl)amino]-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 666702-45-0 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-2-(methylamino)-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{MeNH} & \text{N} & \text{N} \\ \text{N} & \text{N} \\ \text{N} & \text{N} \\ \text{Me} & \text{O} \end{array}$$

RN 666702-50-7 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-2-(cyclohexylamino)-1,7-dihydro-1-methyl-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$NH$$
 $N$ 
 $N$ 
 $N$ 
 $NH_2$ 
 $NH_2$ 
 $NH_2$ 

RN 666702-56-3 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-2-[(cyclohexylmethyl)amino]-1,7-dihydro-1-methyl-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$CH_2-NH$$
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $NH_2$ 
 $CH_2-Ph$ 

RN 666702-63-2 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-2-(dimethylamino)-1,7-dihydro-1-methyl-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 666702-67-6 USPATFULL

CN 6H-Purin-6-one, 2-amino-8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} H_2N & N & N & N \\ \hline Me & O & CH_2-Ph \end{array}$$

RN 666702-70-1 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-7-(3-methyl-2-butenyl)-2-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

RN 666702-73-4 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1,2-dimethyl-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

Me N N N NH2
$$CH_2 - Ph$$

RN 666702-77-8 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-7-(3-methyl-2-butenyl)-2-(2-phenylethyl)- (9CI) (CA INDEX NAME)

RN 666702-82-5 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} N & N & N \\ N & N \\ N & N \\ CH_2-Ph \end{array}$$

RN 666702-86-9 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-2-(methylthio)-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 666702-89-2 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-7-(phenylmethyl)-2-[(phenylmethyl)thio]- (9CI) (CA INDEX NAME)

RN 666702-91-6 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-2-(methylthio)-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{MeS} & \text{N} & \text{N} & \text{N} \\ \hline \text{N} & \text{N} & \text{N} \\ \text{Me} & \text{CH}_2 - \text{Ph} \end{array}$$

RN 666702-94-9 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-2-(methylthio)-1-(2-oxo-2-phenylethyl)-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{MeS} & \text{N} & \text{N} \\ \text{O} & \text{N} & \text{N} \\ \text{Ph-C-CH}_2 & \text{O} & \text{CH}_2-\text{Ph} \end{array}$$

RN 666702-97-2 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-2-(methylthio)-1,7-bis(phenylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{MeS} & \text{N} & \text{N} & \text{N} \\ \text{Ph-CH}_2 & \text{N} & \text{N} & \text{N} \\ \text{O} & \text{CH}_2 - \text{Ph} \end{array}$$

RN 666703-02-2 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-2-(methylthio)-1-(2-phenylethyl)-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 666703-05-5 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-(2-oxo-2-phenylethyl)-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ \text{Ph-} & \text{C-} & \text{CH}_2 \end{array} \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ &$$

666703-09-9 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-2-[[(4-fluorophenyl)methyl]amino]-1,7-dihydro-1-methyl-7-(phenylmethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

RN

CRN 666702-31-4 CMF C25 H28 F N7 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 666703-11-3 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-2-[(2-

phenylethyl)amino]-7-(phenylmethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 666702-35-8 CMF C26 H31 N7 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 666703-14-6 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-2-[(1-methylethyl)amino]-7-(phenylmethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 666702-40-5 CMF C21 H29 N7 O

$$i-PrNH$$
 $N$ 
 $N$ 
 $N$ 
 $NH_2$ 
 $CH_2-Ph$ 

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 666703-17-9 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-2-(methylamino)-7-(phenylmethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 666702-45-0 CMF C19 H25 N7 O

MeNH N N NH2 NH2 
$$\sim$$
 CH2-Ph

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 666703-20-4 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-2-(cyclohexylamino)-1,7-dihydro-1-methyl-7-(phenylmethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 666702-50-7 CMF C24 H33 N7 O

CRN 76-05-1 CMF C2 H F3 O2

RN 666703-21-5 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-2-[(cyclohexylmethyl)amino]-1,7- dihydro-1-methyl-7-(phenylmethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 666702-56-3 CMF C25 H35 N7 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 666703-25-9 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-2-(dimethylamino)-1,7-dihydro-1-methyl-7-(phenylmethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 666702-63-2 CMF C20 H27 N7 O

CRN 76-05-1 CMF C2 H F3 O2

RN 666703-27-1 USPATFULL

CN 6H-Purin-6-one, 2-amino-8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-7-(phenylmethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 666702-67-6 CMF C18 H23 N7 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 666703-29-3 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-7-(3-methyl-2-butenyl)-2-[(phenylmethyl)amino]-, trifluoroacetate (9CI) (CA INDEX

NAME)

CM 1

CRN 666702-70-1 CMF C23 H31 N7 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 666703-31-7 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1,2-dimethyl-7-(phenylmethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 666702-73-4 CMF C19 H24 N6 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 666703-33-9 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-7-(3-methyl-2-butenyl)-2-(2-phenylethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 666702-77-8 CMF C24 H32 N6 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 666703-35-1 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-7-(phenylmethyl)-, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} N & N & N \\ N & N \\ N & N \\ CH_2-Ph \end{array}$$

•x HCl

RN 666703-37-3 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-2-(methylthio)-7-(phenylmethyl)-, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{MeS} & \overset{H}{N} & N \\ \hline & N \\ N \\ & N \\ \end{array}$$

●x HCl

RN 666703-41-9 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-2-(methylthio)-1-(2-oxo-2-phenylethyl)-7-(phenylmethyl)-, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{MeS} & \text{N} & \text{N} \\ \text{O} & \text{N} & \text{N} \\ \text{Ph-C-CH}_2 & \text{O} & \text{CH}_2\text{-Ph} \end{array}$$

•x HCl

RN 666703-45-3 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-2-(methylthio)-1,7-bis(phenylmethyl)-, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{MeS} & \text{N} & \text{N} & \text{N} \\ \text{Ph-CH}_2 & \text{N} & \text{CH}_2 - \text{Ph} \\ \end{array}$$

●x HCl

RN 666703-47-5 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-2-(methylthio)-1-(2-phenylethyl)-7-(phenylmethyl)-, hydrochloride (9CI). (CA INDEX NAME)

$$\begin{array}{c|c} \text{MeS} & \text{N} & \text{N} \\ \text{N} & \text{N} \\ \text{Ph-CH}_2-\text{CH}_2 & \text{O} \\ \end{array}$$

# ●x HCl

RN 666703-50-0 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-7-(phenylmethyl)-2-[(phenylmethyl)thio]-, hydrochloride (9CI) (CA INDEX NAME)

### •x HCl

RN 666703-52-2 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-2-[(2-phenylethyl)thio]-7-(phenylmethyl)-, hydrochloride (9CI) (CA INDEX NAME)

### ●x HCl

RN 666703-54-4 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-(2-oxo-2-phenylethyl)-7-(phenylmethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 666703-05-5 CMF C25 H26 N6 O2

CRN 76-05-1 CMF C2 H F3 O2

RN 666703-56-6 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-7-(phenylmethyl)-2-[(phenylmethyl)thio]-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 666702-89-2 CMF C24 H26 N6 O S

$$Ph$$
- $CH_2$ - $S$ 
 $N$ 
 $N$ 
 $N$ 
 $NH_2$ 
 $CH_2$ - $Ph$ 

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 666704-19-4 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-7-

(phenylmethyl)-2-[(phenylmethyl)amino]-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 666702-26-7 CMF C25 H29 N7 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 666704-74-1 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-1,7-dihydro-1-methyl-2-(methylthio)-7-(phenylmethyl)-, hydrochloride (9CI) (CA INDEX NAME)

MeS N N N NH2 NH2 
$$\sim$$
 CH2-Ph

#### •x HCl

IT 666703-62-4P 666703-64-6P 666703-66-8P 666703-68-0P 666703-74-8P 666703-76-0P 666703-78-2P 666703-80-6P 666703-82-8P 666703-84-0P 666703-86-2P 666703-88-4P 666703-90-8P 666703-92-0P 666703-94-2P 666704-02-5P 666704-04-7P 666704-06-9P 666704-08-1P 666704-09-2P 666704-11-6P 666704-15-0P 666704-15-0P

(preparation of purine derivs. as dipeptidylpeptidase IV inhibitors) RN 666703-62-4 USPATFULL

CN Carbamic acid, [1-[6,7-dihydro-6-oxo-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 666703-64-6 USPATFULL

CN Carbamic acid, [1-[6,7-dihydro-1-methyl-6-oxo-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 666703-66-8 USPATFULL

CN Carbamic acid, [1-[6,7-dihydro-6-oxo-1-(2-oxo-2-phenylethyl)-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 666703-68-0 USPATFULL

CN Carbamic acid, [1-[6,7-dihydro-2-(methylthio)-6-oxo-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{MeS} & \overset{H}{\overset{N}{\overset{}}} & \overset{O}{\overset{}} & \overset{O}{\overset{}} \\ \text{N} & \overset{O}{\overset{}} & \overset{O}{\overset{}} \\ \text{CH}_2-\text{Ph} \end{array}$$

RN 666703-74-8 USPATFULL

CN Carbamic acid, [1-[6,7-dihydro-6-oxo-7-(phenylmethyl)-2-[(phenylmethyl)thio]-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$Ph-CH_2-S$$
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $NH-C-OBu-t$ 
 $CH_2-Ph$ 

- RN 666703-76-0 USPATFULL
- CN Carbamic acid, [1-[6,7-dihydro-2-(methylthio)-6-oxo-7-(2-propenyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

- RN 666703-78-2 USPATFULL
- CN Carbamic acid, [1-[6,7-dihydro-6-oxo-2-[(2-phenylethyl)thio]-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

- RN 666703-80-6 USPATFULL
- CN Carbamic acid, [1-[6,7-dihydro-1-methyl-2-(methylthio)-6-oxo-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 666703-82-8 USPATFULL

CN Carbamic acid, [1-[6,7-dihydro-2-(methylthio)-6-oxo-1-(2-oxo-2-phenylethyl)-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{MeS} & \text{N} & \text{N} \\ \text{O} & \text{N} & \text{N} \\ \text{Ph-C-CH}_2 & \text{N} & \text{N} \\ \text{O} & \text{CH}_2\text{-Ph} \end{array}$$

RN 666703-84-0 USPATFULL

CN Carbamic acid, [1-[6,7-dihydro-1-methyl-7-(3-methyl-2-butenyl)-2-(methylthio)-6-oxo-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 666703-86-2 USPATFULL

CN Carbamic acid, [1-[6,7-dihydro-2-(methylthio)-6-oxo-1,7-bis(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

MeS N N N N NH-C-OBu-t 
$$CH_2-Ph$$

RN 666703-88-4 USPATFULL

CN Carbamic acid, [1-[6,7-dihydro-1-methyl-6-oxo-7-(phenylmethyl)-2-[(phenylmethyl)thio]-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 666703-90-8 USPATFULL

CN Carbamic acid, [1-[6,7-dihydro-1-methyl-6-oxo-2-[(2-phenylethyl)thio]-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$Ph-CH_2-CH_2-S$$
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $NH-C-OBu-t$ 
 $CH_2-Ph$ 

RN 666703-92-0 USPATFULL

CN Carbamic acid, [1-[6,7-dihydro-1-methyl-2-(methylsulfinyl)-6-oxo-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 666703-94-2 USPATFULL

CN Carbamic acid, [1-[6,7-dihydro-1-methyl-2-(methylsulfonyl)-6-oxo-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & & & & \\ Me - S & & N & & N & & \\ \hline O & N & & N & & N \\ Me & & N & & N \\ & & & CH_2-Ph \\ \end{array}$$

RN 666703-96-4 USPATFULL

CN Carbamic acid, [1-[6,7-dihydro-1-methyl-7-(3-methyl-2-butenyl)-2-(methylsulfinyl)-6-oxo-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Me 
$$\stackrel{\circ}{\underset{N}{=}}$$
  $\stackrel{\circ}{\underset{N}{=}}$   $\stackrel{\circ}{\underset{NH-C-OBu-t}{=}}$   $\stackrel{\circ}{\underset{NH-C-OBu-t}{=}}$ 

RN 666703-98-6 USPATFULL

CN Carbamic acid, [1-[6,7-dihydro-1-methyl-6-oxo-7-(phenylmethyl)-2-[(phenylmethyl)amino]-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 666704-00-3 USPATFULL

CN Carbamic acid, [1-[2-[[(4-fluorophenyl)methyl]amino]-6,7-dihydro-1-methyl-6-oxo-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 666704-02-5 USPATFULL

CN Carbamic acid, [1-[6,7-dihydro-1-methyl-6-oxo-2-[(2-phenylethyl)amino]-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 666704-04-7 USPATFULL

CN Carbamic acid, [1-[6,7-dihydro-1-methyl-2-[(1-methylethyl)amino]-6-oxo-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester

# (9CI) (CA INDEX NAME)

RN 666704-06-9 USPATFULL

CN Carbamic acid, [1-[6,7-dihydro-1-methyl-2-(methylamino)-6-oxo-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 666704-08-1 USPATFULL

CN Carbamic acid, [1-[2-(cyclohexylamino)-6,7-dihydro-1-methyl-6-oxo-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 666704-09-2 USPATFULL

CN Carbamic acid, [1-[2-[(cyclohexylmethyl)amino]-6,7-dihydro-1-methyl-6-oxo-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$CH_2-NH$$
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $NH-C-OBu-t$ 
 $CH_2-Ph$ 

RN 666704-11-6 USPATFULL

CN Carbamic acid, [1-[2-(dimethylamino)-6,7-dihydro-1-methyl-6-oxo-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester

# (9CI) (CA INDEX NAME)

RN 666704-12-7 USPATFULL

CN Carbamic acid, [1-[2-amino-6,7-dihydro-1-methyl-6-oxo-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 666704-13-8 USPATFULL

CN Carbamic acid, [1-[6,7-dihydro-1-methyl-7-(3-methyl-2-butenyl)-6-oxo-2-[(phenylmethyl)amino]-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 666704-14-9 USPATFULL

Me N N N N NH-C-OBu-t 
$$CH_2-Ph$$

RN 666704-15-0 USPATFULL

CN Carbamic acid, [1-[6,7-dihydro-1-methyl-7-(3-methyl-2-butenyl)-6-oxo-2-(2-phenylethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester

### (9CI) (CA INDEX NAME)

RN 666704-16-1 USPATFULL

CN Carbamic acid, [1-[6,7-dihydro-2-(methylthio)-6-oxo-1-(2-phenylethyl)-7-(phenylmethyl)-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

L32 ANSWER 14 OF 17 USPATFULL on STN

ACCESSION NUMBER:

2004:152106 USPATFULL

TITLE:

INVENTOR(S):

Condensed imidazole derivatives Yoshikawa, Seiji, Kashima-gun, JAPAN Emori, Eita, Tsuchiura-shi, JAPAN Matsuura, Fumiyoshi, Tsukuba-shi, JAPAN

Matsuura, Fumiyoshi, Tsukuba-shi, JAPAN Clark, Richard, Tsuchiura-shi, JAPAN Ikuta, Hironori, Ushiku-shi, JAPAN Kira, Kazunobu, Tsukuba-shi, JAPAN Yasuda, Nobuyuki, Tsuchiura-shi, JAPAN Nagakura, Tadashi, Ushiku-shi, JAPAN Yamazaki, Kazuto, Tsukuba-shi, JAPAN

PATENT ASSIGNEE(S):

Eisai Co., Ltd., Tokyo, JAPAN (non-U.S. corporation)

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DOCUMENT TYPE: Utility

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LEGAL REPRESENTATIVE: TOWNSEND AND TOWNSEND AND CREW, LLP, TWO EMBARCADERO CENTER, EIGHTH FLOOR, SAN FRANCISCO, CA, 94111-3834

NUMBER OF CLAIMS: 33 EXEMPLARY CLAIM: 1 LINE COUNT: 9667

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The present invention is related to compounds represented by the following formula, or salts or hydrates thereof ##STR1##

wherein,

T.sup.1 represents a 4- to 12-membered heterocyclic group containing one or two nitrogen atoms in the ring, which is a monocyclic or bicyclic structure that may have one or more substituents;

X represents a C.sub.1-6 alkyl group which may have one or more substituents, or such;

Z.sup.1 and Z.sup.2 each independently represent a nitrogen atom or a
group represented by the formula --CR.sup.2--;

R.sup.1 and R.sup.2 independently represent a hydrogen atom, a C.sub.1-6 alkyl group which may have one or more substituents, or a C.sub.1-6 alkoxy group which may have one or more substituents, or such.

These are novel compounds that exhibit an excellent DPPIV-inhibiting activity.

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CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT 635715-41-2P 635715-43-4P 635715-48-9P
      635715-52-5P 635715-57-0P 635715-58-1P
     635715-60-5P 635715-62-7P 635715-63-8P
     635715-64-9P 635715-66-1P 635715-68-3P
     635715-79-6P 635715-81-0P 635715-83-2P
     635715-85-4P 635715-87-6P 635715-91-2P
     635715-93-4P 635715-95-6P 635715-97-8P
     635715-99-0P 635716-01-7P 635716-05-1P
     635716-09-5P 635716-11-9P 635716-13-1P
     635716-15-3P 635716-17-5P 635716-19-7P
     635716-23-3P 635716-27-7P 635716-29-9P
     635716-31-3P 635716-33-5P 635716-35-7P
     635716-39-1P 635716-45-9P 635716-47-1P
     635716-53-9P 635716-55-1P 635716-57-3P
      635716-59-5P 635716-65-3P 635716-67-5P
     635716-69-7P 635716-71-1P 635716-73-3P
      635716-75-5P 635716-77-7P 635716-79-9P
      635716-81-3P 635716-86-8P 635716-90-4P
     635716-93-7P 635717-00-9P 635717-02-1P
     635717-05-4P 635717-08-7P 635717-10-1P
     635717-13-4P 635717-16-7P 635717-18-9P
      635717-20-3P 635717-22-5P 635717-24-7P
      635717-25-8P 635717-26-9P 635717-28-1P
      635717-30-5P 635717-32-7P 635717-35-0P
     635717-36-1P 635717-37-2P 635717-39-4P
     635717-41-8P 635717-43-0P 635717-45-2P
     635717-46-3P 635717-47-4P 635717-48-5P
     635717-49-6P 635717-50-9P 635717-51-0P
     635717-53-2P 635717-55-4P 635717-57-6P
     635717-59-8P 635717-61-2P 635717-63-4P
     635717-84-9P 635717-86-1P 635717-90-7P
     635717-93-0P 635717-96-3P 635717-99-6P
     635718-02-4P 635718-08-0P 635718-10-4P
     635718-21-7P 635718-23-9P 635718-25-1P
     635718-33-1P 635718-35-3P 635718-37-5P
     635718-39-7P 635718-59-1P 635718-71-7P
     635718-73-9P 635718-77-3P 635718-79-5P
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635719-41-4P 635719-45-8P 635719-47-0P
      635719-53-8P 635719-57-2P 635719-73-2P
      635719-77-6P 635719-79-8P 635719-81-2P
      635719-83-4P 635719-85-6P 635719-87-8P
      635719-89-0P 635719-91-4P 635719-93-6P
      635719-95-8P 635719-97-0P 635720-02-4P
      635720-16-0P 635720-18-2P 635720-22-8P
      635720-25-1P 635720-26-2P 635720-27-3P
      635720-28-4P 635720-29-5P 635720-30-8P
      635720-34-2P 635720-36-4P 635720-38-6P
      635720-40-0P 635720-43-3P 635720-45-5P
        (preparation of purinone derivs. as dipeptidylpeptidase IV inhibitors)
RN
     635715-41-2 USPATFULL
CN
     Acetic acid, [[7-(2-chlorophenyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-
       piperazinyl)-1H-purin-2-yl]oxy]-, ethyl ester, mono(trifluoroacetate)
              (CA INDEX NAME)
     CM
          1
     CRN
          635715-40-1
     CMF
          C20 H23 Cl N6 O4
```

CRN 76-05-1 CMF C2 H F3 O2

CRN 635715-42-3 CMF C18 H19 C1 N6 O4

CRN 76-05-1 CMF C2 H F3 O2

RN 635715-48-9 USPATFULL

CN Benzeneacetic acid,  $\alpha$ -[[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]oxy]-, methyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-47-8 CMF C23 H26 N6 O4

MeO-C-CH-O N N N N N N N N 
$$\sim$$
 CH<sub>2</sub>-C $\rightleftharpoons$  C-Me

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635715-52-5 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-(1-methylpropoxy)-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-51-4 CMF C18 H26 N6 O2

$$\begin{array}{c|c} \text{Me} & & & \\ \text{Et-CH-O} & & & & \\ \text{N} & & & & \\ \text{Me} & & & & \\ \text{N} & & & & \\ \text{O} & & & & \\ \text{CH}_2-\text{C} & & \\ \text{C-Me} \end{array}$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635715-57-0 USPATFULL

CN Butanoic acid, 2-[[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]oxy]-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-56-9 CMF C20 H28 N6 O4

CRN 76-05-1 CMF C2 H F3 O2

RN 635715-58-1 USPATFULL

CN Propanoic acid, 2-[[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]oxy]-, ethyl ester (9CI) (CA INDEX NAME)

EtO-C-CH-ONNNNNH

Me

$$NH$$
 $CH_2-C$ 
 $C-Me$ 

RN 635715-60-5 USPATFULL

CN Propanoic acid, 2-[[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]oxy]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-59-2 CMF C17 H22 N6 O4

$$\begin{array}{c|c} \text{Me} & & & \\ \text{HO}_2\text{C}-\text{CH}-\text{O} & & & \\ \text{N} & & & \\ \text{CH}_2-\text{C} & & \\ \text{C}-\text{Me} & & \\ \end{array}$$

CRN 76-05-1 CMF C2 H F3 O2

RN 635715-62-7 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-2-methoxy-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-61-6 CMF C15 H20 N6 O2

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635715-63-8 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-2-ethoxy-1,7-dihydro-1-methyl-8-(1-

piperazinyl) - (9CI) (CA INDEX NAME)

RN 635715-64-9 USPATFULL

CN Acetic acid, [[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]oxy]-, ethyl ester (9CI) (CA INDEX NAME)

RN 635715-66-1 USPATFULL

CN Acetic acid, [[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]oxy]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-65-0 CMF C16 H20 N6 O4

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635715-68-3 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-2-(2-methoxyethoxy)-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-67-2 CMF C17 H24 N6 O3

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635715-79-6 USPATFULL

CN 1H-Purine-2-acetic acid, 7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-78-5 CMF C18 H24 N6 O3

EtO-C-CH<sub>2</sub>
N
N
N
N
$$CH_2$$
-C=C-Me

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635715-81-0 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1,2-dimethyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-80-9 CMF C15 H20 N6 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635715-83-2 USPATFULL

CN 6H-Purin-6-one, 2-butyl-7-(2-butynyl)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-82-1 CMF C18 H26 N6 O

CRN 76-05-1 CMF C2 H F3 O2

RN 635715-85-4 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-(phenylmethyl)-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-84-3 CMF C21 H24 N6 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635715-87-6 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-(2-phenylethyl)-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-86-5 CMF C22 H26 N6 O

Ph-CH<sub>2</sub>-CH<sub>2</sub>
N
N
N
N
N
$$CH_2$$
-C
 $C$ -Me

CRN 76-05-1 CMF C2 H F3 O2

RN 635715-91-2 USPATFULL

CN 6H-Purin-6-one, 2-amino-7-(2-butynyl)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-90-1 CMF C14 H19 N7 O

$$\begin{array}{c|c} H_2N & N & N & NH \\ \hline N & N & N & NH \\ \hline Me & CH_2-C = C-Me \end{array}$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635715-93-4 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-(methylamino)-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 635715-92-3 CMF C15 H21 N7 O

MeNH N N N N N 
$$\sim$$
 CH<sub>2</sub> - C  $\sim$  C  $\sim$  Me

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635715-95-6 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-2-(dimethylamino)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-94-5 CMF C16 H23 N7 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635715-97-8 USPATFULL

CN Glycine, N-[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-96-7 CMF C18 H25 N7 O3

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635715-99-0 USPATFULL

CN Glycine, N-[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635715-98-9 CMF C16 H21 N7 O3

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-01-7 USPATFULL

CN Glycine, N-[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]-N-methyl-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-00-6 CMF C19 H27 N7 O3

$$\begin{array}{c|c} O & Me \\ \parallel & \parallel & \parallel \\ EtO-C-CH_2-N & N & N & NH \\ \hline Me & N & N & NH \\ \hline Me & N & NH \\ \hline & NH & N$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-05-1 USPATFULL

CN Glycine, N-[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]-N-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-04-0 CMF C17 H23 N7 O3

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-09-5 USPATFULL
CN Alanine, N-[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1Hpurin-2-yl]-, methyl ester, mono(trifluoroacetate) (9CI) (CA INDEX
NAME)

CM 1

CRN 635716-08-4 CMF C18 H25 N7 O3

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-11-9 USPATFULL

CN Alanine, N-[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]-2-methyl-, methyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-10-8 CMF C19 H27 N7 O3

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-13-1 USPATFULL

CN L-Alanine, N-[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-12-0 CMF C19 H27 N7 O3

Absolute stereochemistry.

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-15-3 USPATFULL

CN L-Alanine, N-[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-14-2 CMF C17 H23 N7 O3

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-17-5 USPATFULL
CN β-Alanine, N-[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-16-4 CMF C19 H27 N7 O3

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-19-7 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-2-[(2-ethoxyethyl)amino]-1,7-dihydro-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-18-6 CMF C18 H27 N7 O2

EtO-
$$CH_2$$
- $CH_2$ - $NH$ 

N

N

N

 $CH_2$ - $C$ 
 $C$ 
 $C$ 
 $C$ 
 $C$ 
 $C$ 

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-23-3 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-[(phenylmethyl)amino]-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-22-2 CMF C21 H25 N7 O

Ph-CH<sub>2</sub>-NH NH NH NH 
$$\sim$$
 NH  $\sim$  NH

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-27-7 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2[methyl (phenylmethyl) amino]-8-(1-piperazinyl)-, mono(trifluoroacetate)
(9CI) (CA INDEX NAME)

CM 1

CRN 635716-26-6 CMF C22 H27 N7 O

$$\begin{array}{c|c} \text{Me} & & & \text{NH} \\ \text{Ph-} \text{CH}_2 - \text{N} & & & \text{NH} \\ \text{Me} & & & \text{N} & & \\ \text{Me} & & & \text{CH}_2 - \text{C} = \text{C-Me} \end{array}$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

CM 1

CRN 635716-28-8 CMF C21 H24 Cl N7 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-31-3 USPATFULL CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-2-[[(4-methoxyphenyl)methyl]amino]-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-30-2 CMF C22 H27 N7 O2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-33-5 USPATFULL CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-[(2-phenylethyl)amino]-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-32-4 CMF C22 H27 N7 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-35-7 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-[methyl(2-phenylethyl)amino]-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-34-6 CMF C23 H29 N7 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-39-1 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-2-[(2-pyridinylmethyl)amino]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-38-0 CMF C20 H24 N8 O

CM 2

RN 635716-45-9 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-2-(diethylamino)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-44-8 CMF C18 H27 N7 O

$$\begin{array}{c|c} \text{Et}_2 \text{N} & \text{N} & \text{N} \\ \text{Me} & \text{N} & \text{N} & \text{N} \\ \text{O} & \text{CH}_2 - \text{C} = \text{C} - \text{Me} \end{array}$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-47-1 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-2-(ethylmethylamino)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-46-0 CMF C17 H25 N7 O

$$\begin{array}{c|c} \text{Me} & & & \\ \hline Et-N & N & N & N \\ \hline Me & & N & N \\ \hline & & CH_2-C \end{array} \subset C-Me$$

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-53-9 USPATFULL

CN Acetonitrile, [[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]methylamino]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-52-8 CMF C17 H22 N8 O

$$\begin{array}{c|c} \text{Me} & & & \text{NH} \\ \text{NC-CH}_2-\text{N} & & & \text{N} \\ \text{Me} & & & \text{N} \\ & & & \text{CH}_2-\text{C} \end{array} \subset \text{Me}$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-55-1 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-[(1-methylethyl)amino]-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-54-0 CMF C17 H25 N7 O

i-PrNH N N N N N 
$$\sim$$
 NH  $\sim$  NH  $\sim$  NH  $\sim$  CH<sub>2</sub>-C $\sim$  C-Me

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-57-3 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-2-(2-pyridinylamino)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-56-2 CMF C19 H22 N8 O

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-59-5 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-(phenylamino)-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 635716-58-4 CMF C20 H23 N7 O

PhNH N N N N N N N N N N N CH2-C 
$$=$$
 C-Me

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-65-3 USPATFULL

CN Alanine, N-[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-64-2 CMF C17 H23 N7 O3

$$\begin{array}{c|c} \text{Me} & & & \\ \text{HO}_2\text{C}-\text{CH}-\text{NH} & & & \\ \text{N} & & & \\ \text{O} & & & \\ \text{CH}_2-\text{C} \Longrightarrow \text{C}-\text{Me} \end{array}$$

CM 2

RN 635716-67-5 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-2-(2-pyridinylmethoxy)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-66-4 CMF C20 H23 N7 O2

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-69-7 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-(1-methylethoxy)-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-68-6 CMF C17 H24 N6 O2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-71-1 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-2-(2-butynyloxy)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-70-0 CMF C18 H22 N6 O2

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-73-3 USPATFULL

CN Acetic acid, [[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]thio]-, methyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-72-2 CMF C17 H22 N6 O3 S

MeO-C-CH<sub>2</sub>-S
N
N
N
N
$$CH_2$$
-C=C-Me

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-75-5 USPATFULL
CN Propanoic acid, 2-[[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]thio]-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-74-4 CMF C19 H26 N6 O3 S

CM 2

RN 635716-77-7 USPATFULL

CN Propanoic acid, 3-[[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]thio]-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-76-6 CMF C19 H26 N6 O3 S

EtO-C-CH<sub>2</sub>-CH<sub>2</sub>-S
N
N
N
N
$$CH_2$$
-C
 $C$ -Me

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-79-9 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-2-(ethylthio)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-78-8 CMF C16 H22 N6 O S

EtS N N N N N N N N 
$$\sim$$
 CH<sub>2</sub>-C $\Longrightarrow$  C-Me

CM 2

RN 635716-81-3 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-2-[(2-hydroxyethyl)thio]-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-80-2 CMF C16 H22 N6 O2 S

HO- 
$$CH_2$$
-  $CH_2$ -  $S$ 

N
N
N
N
 $CH_2$ -  $C$ 
 $C$ 
 $C$ 
 $C$ 

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-86-8 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-(methylthio)-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-85-7 CMF C15 H20 N6 O S

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-90-4 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-[(1-methylethyl)thio]-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-89-1 CMF C17 H24 N6 O S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635716-93-7 USPATFULL

N 6H-Purin-6-one, 7-(2-butynyl)-2-[(1,1-dimethylethyl)thio]-1,7-dihydro-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-92-6 CMF C18 H26 N6 O S

CRN 76-05-1 CMF C2 H F3 O2

RN 635717-00-9 USPATFULL

CN Acetic acid, [[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]thio]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635716-99-3 CMF C16 H20 N6 O3 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635717-02-1 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-2-(ethylsulfinyl)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 635717-01-0 CMF C16 H22 N6 O2 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635717-05-4 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-2-(ethylsulfonyl)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635717-04-3 CMF C16 H22 N6 O3 S

$$\begin{array}{c|c} C & NH \\ \hline C & NH \\ \hline O & N \\ \hline Me & CH_2-C \end{array}$$

CM 2

RN 635717-08-7 USPATFULL

CN 1H-Purine-2-carbonitrile, 7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635717-07-6 CMF C15 H17 N7 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635717-10-1 USPATFULL

CN 1H-Purine-2-carboxamide, 7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
O & & & & & & \\
H_2N-C & & N & & N & & NH \\
\hline
N & & & N & & N & & NH \\
Me & & & N & & N & & NH
\end{array}$$

$$CH_2-C \Longrightarrow C-Me$$

RN 635717-13-4 USPATFULL

CN 1H-Purine-2-carboxylic acid, 7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 635717-12-3 CMF C15 H18 N6 O3

$$\begin{array}{c|c} \text{HO}_2\text{C} & \text{N} & \text{N} \\ \text{Me} & \text{N} & \text{N} \\ \text{O} & \text{CH}_2\text{--}\text{C} \end{array} \text{C--Me}$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

CM 1

CRN 635717-15-6 CMF C14 H18 N6 O

CM 2

RN 635717-18-9 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-2-methoxy-1-(2-phenylethyl)-8-(1-piperazinyl)-, monohydrochloride (9CI) (CA INDEX NAME)

### HCl

RN 635717-20-3 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-2-ethoxy-1,7-dihydro-1-(2-phenylethyl)-8-(1-piperazinyl)-, monohydrochloride (9CI) (CA INDEX NAME)

Ph-CH<sub>2</sub>-CH<sub>2</sub> 
$$\stackrel{N}{\longrightarrow}$$
  $\stackrel{N}{\longrightarrow}$   $\stackrel{N}{\longrightarrow}$ 

#### HCl

RN 635717-22-5 USPATFULL

MeO-C-CH<sub>2</sub>-S
N
N
N
N
N
N
$$CH_2$$
-C=C-Me

RN 635717-24-7 USPATFULL
CN Glycine, N-[7-(2-butynyl)-6,7-dihydro-6-oxo-1-(2-phenylethyl)-8-(1-piperazinyl)-1H-purin-2-yl]-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O \\ \hline \\ EtO-C-CH_2-NH \\ \hline \\ Ph-CH_2-CH_2 \\ \hline \\ O \end{array} \begin{array}{c} NH \\ \hline \\ N \\ \hline \\ CH_2-C \end{array} \begin{array}{c} C-Me \\ \hline \end{array}$$

### ● HCl

RN 635717-25-8 USPATFULL
CN Acetamide, 2-[[7-(2-butynyl)-1,7-dihydro-6-oxo-1-(2-phenylethyl)-8-(1-piperazinyl)-1H-purin-2-yl]amino]-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O \\ H_2N-C-CH_2-NH \\ Ph-CH_2-CH_2 \\ \end{array} \begin{array}{c} NH \\ N \\ O \\ \end{array} \begin{array}{c} NH \\ CH_2-C \Longrightarrow C-Me \\ \end{array}$$

## ● HCl

RN 635717-26-9 USPATFULL
CN Glycine, N-[7-(2-butynyl)-6,7-dihydro-6-oxo-1-(2-phenylethyl)-8-(1-piperazinyl)-1H-purin-2-yl]-N-methyl-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & \text{Me} \\ \parallel & \parallel & \parallel \\ \text{EtO-C-CH}_2 - N & N & N \\ \text{Ph-CH}_2 - \text{CH}_2 & & N \\ \end{array}$$

RN 635717-28-1 USPATFULL

CN Acetic acid, [[7-(2-butynyl)-6,7-dihydro-6-oxo-1-(2-phenylethyl)-8-(1-piperazinyl)-1H-purin-2-yl]oxy]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

### ● HCl

RN 635717-30-5 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-2-(2-hydroxyethoxy)-1-(2-phenylethyl)-8-(1-piperazinyl)-, monohydrochloride (9CI) (CA INDEX NAME)

# HCl

RN 635717-32-7 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-2-(dimethylamino)-1,7-dihydro-1-(2-phenylethyl)-8-(1-piperazinyl)-, monohydrochloride (9CI) (CA INDEX NAME)

RN 635717-35-0 USPATFULL

CN Benzonitrile, 2-[[7-(2-butynyl)-2-(dimethylamino)-6,7-dihydro-6-oxo-8-(1-piperazinyl)-1H-purin-1-yl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me-}\text{C} & \text{C-}\text{CH}_2 \\ \hline \text{CN} & \text{O} \\ \hline \text{CH}_2 & \text{N} \\ \hline \text{Me}_2 \text{N} & \text{N} \end{array}$$

### ● HCl

RN 635717-36-1 USPATFULL

CN Acetic acid, [[7-(2-butyny1)-1-[(2-cyanophenyl)methyl]-6,7-dihydro-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]thio]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me-}\text{C} & \text{C-}\text{CH}_2 \\ \hline & \text{CN} & \text{O} \\ \hline & \text{CH}_2 & \text{N} \\ \hline & \text{N} & \text{N} \\ \\ \text{MeO-}\text{C-}\text{CH}_2 - \text{S} \\ \end{array}$$

## ● HCl

RN 635717-37-2 USPATFULL

CN Benzonitrile, 2-[[7-(2-butynyl)-6,7-dihydro-2-methoxy-6-oxo-8-(1-piperazinyl)-1H-purin-1-yl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me-C} \subset \text{C-CH}_2 \\ \text{CN} & \text{O} \\ \text{CH}_2 & \text{N} & \text{N} \\ \text{MeO} & \text{N} & \text{N} \end{array}$$

RN 635717-39-4 USPATFULL

CN Acetic acid, [[7-(2-butynyl)-1-(cyanomethyl)-6,7-dihydro-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]thio]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HCl

RN 635717-41-8 USPATFULL

CN Acetic acid, [[1,7-di-2-butynyl-6,7-dihydro-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]thio]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

MeO-C-CH<sub>2</sub>-S
N
N
N
N
N
N
N
$$CH_2$$
-C
 $C$ -Me

HCl

RN 635717-43-0 USPATFULL

CN 1H-Purine-2-carbonitrile, 1,7-di-2-butynyl-6,7-dihydro-6-oxo-8-(1-piperazinyl)-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{Me-C} & & & \\ \hline \\ \text{C} & & \\ \text{C} & & \\ \end{array} \begin{array}{c} & & \\ \text{N} & \\ \\ \text{N} & \\ \\ \text{C} & \\ \end{array} \begin{array}{c} & \\ \text{NH} \\ \\ \text{C} & \\ \end{array} \begin{array}{c} & \\ \end{array} \begin{array}{c} & \\ \\ \end{array} \begin{array}{c} & \\ & \\ \end{array} \begin{array}{c} & \\ & \\ \end{array} \begin{array}{c} & \\ \\ \end{array} \begin{array}{c} & \\$$

RN 635717-45-2 USPATFULL

CN 6H-Purin-6-one, 1,7-di-2-butynyl-1,7-dihydro-2-methoxy-8-(1-piperazinyl)-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{MeO} & \text{N} & \text{N} & \text{NH} \\ \text{Me-C} & \text{C-CH}_2 & \text{CH}_2 - \text{C} & \text{C-Me} \end{array}$$

#### HCl

RN 635717-46-3 USPATFULL

CN Acetic acid, [[7-(2-butynyl)-6,7-dihydro-6-oxo-8-(1-piperazinyl)-1-(2-propenyl)-1H-purin-2-yl]thio]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

#### ● HCl

RN 635717-47-4 USPATFULL

CN 1H-Purine-2-carbonitrile, 7-(2-butynyl)-6,7-dihydro-6-oxo-8-(1-piperazinyl)-1-(2-propenyl)-, monohydrochloride (9CI) (CA INDEX NAME)

RN 635717-48-5 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-2-methoxy-8-(1-piperazinyl)-1-(2-propenyl)-, monohydrochloride (9CI) (CA INDEX NAME)

### ● HCl

RN 635717-49-6 USPATFULL
CN Acetic acid, [[7-(2-butynyl)-6,7-dihydro-1-(2-methoxyethyl)-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]thio]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

MeO-
$$CH_2$$
- $CH_2$ - $CH_$ 

## HC1

RN 635717-50-9 USPATFULL

CN 1H-Purine-2-carbonitrile, 7-(2-butynyl)-6,7-dihydro-1-(2-methoxyethyl)-6-oxo-8-(1-piperazinyl)-, monohydrochloride (9CI) (CA INDEX NAME)

MeO-
$$CH_2$$
- $CH_2$ 
O
 $CH_2$ - $C$ 
 $C$ 
Me

RN 635717-51-0 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-2-methoxy-1-(2-methoxyethyl)-8-(1-piperazinyl)-, monohydrochloride (9CI) (CA INDEX NAME)

MeO-
$$_{\mathrm{CH_2}-\mathrm{CH_2}}$$
 CH2- $_{\mathrm{C}}$  C-Me

## ● HCl

RN 635717-53-2 USPATFULL

CN 6H-Purin-6-one, 1,7-dihydro-1-methyl-7-(phenylmethyl)-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635717-52-1 CMF C17 H20 N6 O

CM 2

RN 635717-55-4 USPATFULL

CN 6H-Purin-6-one, 1-ethyl-1,7-dihydro-7-(phenylmethyl)-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635717-54-3 CMF C18 H22 N6 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635717-57-6 USPATFULL

CN 1H-Purine-1-acetic acid, 6,7-dihydro-6-oxo-7-(phenylmethyl)-8-(1-piperazinyl)-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635717-56-5 CMF C20 H24 N6 O3

CRN 76-05-1 CMF C2 H F3 O2

RN 635717-59-8 USPATFULL

CN 6H-Purin-6-one, 1,7-dihydro-1-(2-methoxyethyl)-7-(phenylmethyl)-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635717-58-7 CMF C19 H24 N6 O2

$$\begin{array}{c|c} & & & \\ & & & \\ \text{MeO-CH}_2\text{-CH}_2 & & \\ & & & \\ & & & \\ \text{O} & & \\ \end{array}$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635717-61-2 USPATFULL

CN 6H-Purin-6-one, 1,7-dihydro-7-(phenylmethyl)-8-(1-piperazinyl)-1-(2-propynyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635717-60-1 CMF C19 H20 N6 O

CRN 76-05-1 CMF C2 H F3 O2

RN 635717-63-4 USPATFULL

CN 1H-Purine-1-acetonitrile, 6,7-dihydro-6-oxo-7-(phenylmethyl)-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635717-62-3 CMF C18 H19 N7 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635717-84-9 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-2-[(3-hydroxypropyl)thio]-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (salt) (9CI) (CA

INDEX NAME)

CM 1

CRN 635717-83-8 CMF C17 H24 N6 O2 S

HO- 
$$(CH_2)_3$$
-S
N
N
N
CH2-C=C-Me

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635717-86-1 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-2-[(2-hydroxypropyl)thio]-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 635717-85-0 CMF C17 H24 N6 O2 S

CM 2

RN 635717-90-7 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-2-[(2,3-dihydroxypropyl)thio]-1,7-dihydro-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 635717-89-4 CMF C17 H24 N6 O3 S

HO- 
$$CH_2$$
-  $CH$ -  $CH_2$ -  $S$ 

Me

NH

 $CH_2$ -  $C$ 
 $C$ 
 $C$ 
 $C$ 
 $C$ 

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635717-93-0 USPATFULL

CN Propanoic acid, 3-[[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]thio]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635717-92-9 CMF C17 H22 N6 O3 S

CRN 76-05-1 CMF C2 H F3 O2

RN 635717-96-3 USPATFULL
CN Propanoic acid, 2-[[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]thio]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635717-95-2 CMF C17 H22 N6 O3 S

$$\begin{array}{c|c} \text{Me} & & & \\ \text{HO}_2\text{C}-\text{CH}-\text{S} & & & \\ \text{N} & & & \\ \text{CH}_2-\text{C} & & \\ \text{C}-\text{Me} \end{array}$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635717-99-6 USPATFULL

CM 1

CRN 635717-98-5 CMF C18 H26 N6 O S

$$\begin{array}{c|c} \text{Me} & & & \\ \text{Et-CH-S} & & & \text{N} & \\ & & & & \\ \text{Me} & & & & \\ & & & & \\ \text{O} & & & & \\ & & & & \\ \end{array}$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635718-02-4 USPATFULL CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-2-(propylthio)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635718-01-3 CMF C17 H24 N6 O S

CM 2

RN 635718-08-0 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-2-(dodecylthio)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635718-07-9 CMF C26 H42 N6 O S

Me- 
$$(CH_2)_{11}$$
-S

N

N

N

CH<sub>2</sub>-C=C-Me

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635718-10-4 USPATFULL

CN 6H-Purin-6-one, 2-[(2-aminoethyl)thio]-7-(2-butynyl)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635718-09-1 CMF C16 H23 N7 O S

CRN 76-05-1 CMF C2 H F3 O2

RN 635718-21-7 USPATFULL

CN L-Cysteine, S-[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635718-20-6 CMF C17 H23 N7 O3 S

Absolute stereochemistry.

$$NH_2$$
 $NH_2$ 
 $NH_2$ 

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635718-23-9 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-[(2-methylpropyl)thio]-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635718-22-8 CMF C18 H26 N6 O S

CRN 76-05-1 CMF C2 H F3 O2

RN 635718-25-1 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-2-[(1,2-dimethylpropyl)thio]-1,7-dihydro-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635718-24-0 CMF C19 H28 N6 O S

$$\begin{array}{c|c} Me & & & & \\ i\text{-Pr-CH-S} & N & N & N \\ \hline & N & N & N$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635718-33-1 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-2-[(2-furanylmethyl)thio]-1,7-dihydro-1-

methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635718-32-0 CMF C19 H22 N6 O2 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635718-35-3 USPATFULL

CN Acetamide, 2-[[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]thio]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635718-34-2 CMF C16 H21 N7 O2 S

CM 2

RN 635718-37-5 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-2-[(2-thienylmethyl)thio]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635718-36-4 CMF C19 H22 N6 O S2

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635718-39-7 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-2-[[1-(2-thienyl)ethyl]thio]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635718-38-6 CMF C20 H24 N6 O S2

CRN 76-05-1 CMF C2 H F3 O2

RN 635718-59-1 USPATFULL Acetamide, N-[2-[[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-CNpiperazinyl) -1H-purin-2-yl]thio]ethyl] -, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM1

CRN 635718-58-0 CMF C18 H25 N7 O2 S

CM2

CRN 76-05-1 C2 H F3 O2 CMF

RN 635718-71-7 USPATFULL CN

6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-8-(1-piperazinyl)-2-(2propenylthio) -, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635718-70-6 C17 H22 N6 O S CMF

CRN 76-05-1 CMF C2 H F3 O2

RN 635718-73-9 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-[[3-(methylthio)phenyl]amino]-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635718-72-8 CMF C21 H25 N7 O S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635718-77-3 USPATFULL

CN Propanoic acid, 2-[[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]thio]-2-methyl-, mono(trifluoroacetate) (9CI)

(CA INDEX NAME)

CM 1

CRN 635718-76-2 CMF C18 H24 N6 O3 S

$$\begin{array}{c|c} \text{Me} & & & \\ \text{HO}_2\text{C}-\text{C}-\text{S} & & & \\ \text{Me} & & & & \\ \text{Me} & & & & \\ \text{Me} & & & & \\ \text{O} & & & & \\ \text{CH}_2-\text{C} = \text{C}-\text{Me} \end{array}$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635718-79-5 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-[methyl(1-methylethyl)amino]-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635718-78-4 CMF C18 H27 N7 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635719-41-4 USPATFULL

CN 3-Pyridinecarboxamide, 6-[[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]amino]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635719-40-3 CMF C20 H23 N9 O2

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635719-45-8 USPATFULL

CN Benzamide, 2-[[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]amino]-N-(1,1-dimethylethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635719-44-7 CMF C25 H32 N8 O2

CRN 76-05-1 CMF C2 H F3 O2

RN 635719-47-0 USPATFULL

CN Benzamide, 2-[[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]amino]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635719-46-9 CMF C21 H24 N8 O2

$$\begin{array}{c|c} O & & & \\ \hline C-NH_2 & & & NH \\ \hline NH & N & N & N \\ \hline Ne & NH & N & NH \\ \hline \\ CH_2-C \Longrightarrow C-Me \\ \end{array}$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635719-53-8 USPATFULL
CN Benzoic acid, 2-[[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]methylamino]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635719-52-7 CMF C22 H25 N7 O3

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635719-57-2 USPATFULL

CN Benzenesulfonamide, 2-[[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]amino]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635719-56-1 CMF C20 H24 N8 O3 S

NH2

NH
NH
NH
NH
NH
NH
NH
CH2-C
$$=$$
 C-Me

CRN 76-05-1 CMF C2 H F3 O2

RN 635719-73-2 USPATFULL
CN 1H-Purine-2-acetonitrile, 7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635719-72-1 CMF C16 H19 N7 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635719-77-6 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-(2-oxopropyl)-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635719-76-5 CMF C17 H22 N6 O2

Me-C-CH<sub>2</sub>
N
N
N
N
$$CH_2$$
C-Me

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635719-79-8 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-2-ethynyl-1,7-dihydro-1-methyl-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635719-78-7 CMF C16 H18 N6 O

HC 
$$\subset$$
 C  $\sim$  N  $\sim$  N  $\sim$  NH  $\sim$  NH  $\sim$  NH  $\sim$  CH<sub>2</sub>-C  $\subset$  C-Me

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635719-81-2 USPATFULL CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-1-methyl-2-[(1-

methylethyl)sulfinyl]-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635719-80-1 CMF C17 H24 N6 O2 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635719-83-4 USPATFULL

CN Acetamide, N-acetyl-N-[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635719-82-3 CMF C18 H23 N7 O3

CRN 76-05-1 CMF C2 H F3 O2

RN 635719-85-6 USPATFULL

CN Acetamide, N-[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635719-84-5 CMF C16 H21 N7 O2

Acnh N N N N N 
$$\sim$$
 CH<sub>2</sub>-C $\equiv$  C-Me

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635719-87-8 USPATFULL

CN Acetonitrile, [[7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]oxy]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 635719-86-7 CMF C16 H19 N7 O2

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635719-89-0 USPATFULL

CN Guanidine, [7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)-1H-purin-2-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635719-88-9 CMF C15 H21 N9 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635719-91-4 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-2-(methylthio)-8-(1-piperazinyl), mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635719-90-3 CMF C14 H18 N6 O S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635719-93-6 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-1,7-dihydro-2-[(1-methylethyl)thio]-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635719-92-5 CMF C16 H22 N6 O S

$$\begin{array}{c|c} i\text{-PrS} & \overset{H}{N} & \overset{N}{N} & \overset{NH}{N} \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ &$$

CRN 76-05-1 CMF C2 H F3 O2

RN 635719-95-8 USPATFULL

CN 6H-Purin-6-one, 7-(2-butynyl)-2-[(1,1-dimethylethyl)thio]-1,7-dihydro-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635719-94-7 CMF C17 H24 N6 O S

t-BuS 
$$\stackrel{H}{\underset{N}{\bigvee}}$$
  $\stackrel{N}{\underset{N}{\bigvee}}$   $\stackrel{N}{\underset{N}{\bigvee}}$   $\stackrel{N}{\underset{N}{\bigvee}}$   $\stackrel{N}{\underset{N}{\bigvee}}$   $\stackrel{N}{\underset{N}{\bigvee}}$   $\stackrel{N}{\underset{N}{\bigvee}}$   $\stackrel{N}{\underset{N}{\bigvee}}$   $\stackrel{N}{\underset{N}{\bigvee}}$   $\stackrel{N}{\underset{N}{\bigvee}}$ 

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635719-97-0 USPATFULL

CN 1H-Purine-2-carbonitrile, 7-(2-butynyl)-6,7-dihydro-6-oxo-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635719-96-9 CMF C14 H15 N7 O

CRN 76-05-1 CMF C2 H F3 O2

RN 635720-02-4 USPATFULL

CN 1H-Purine-2-carbonitrile, 7-(2-butynyl)-1-[(2-cyanophenyl)methyl]-6,7-dihydro-6-oxo-8-(1-piperazinyl)-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 635720-16-0 USPATFULL

CN 1H-Purine-2-carbonitrile, 7-(2-butynyl)-1-[(4-cyanophenyl)methyl]-6,7-dihydro-6-oxo-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635720-15-9 CMF C22 H20 N8 O

$$\begin{array}{c|c} \text{Me-C} & \text{C-CH}_2 \\ \text{NC} & \text{N} & \text{N} \\ \\ \text{NC} & \text{N} & \text{N} \end{array}$$

CRN 76-05-1 CMF C2 H F3 O2

RN 635720-18-2 USPATFULL

CM 1

CRN 635720-17-1 CMF C22 H23 N7 O S

$$\begin{array}{c|c} \text{Me-}\text{C} & \text{C-}\text{CH}_2 \\ \text{O} & \text{N} \\ \text{CH}_2 & \text{N} & \text{N} \\ \text{MeS} & \text{N} \end{array}$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635720-22-8 USPATFULL

CN 1H-Purine-2-carbonitrile, 7-(2-butynyl)-1-[(3-cyanophenyl)methyl]-6,7-

dihydro-6-oxo-8-(1-piperazinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635720-21-7 CMF C22 H20 N8 O

$$\begin{array}{c|c} & CH_2-C \\\hline \\ NC \\\hline \\ NC \\\hline \end{array} \begin{array}{c|c} CH_2-C \\\hline \\ N \\\hline \end{array} \begin{array}{c} CH_2-N \\\hline \\ N \\\hline \end{array}$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635720-25-1 USPATFULL

CN 1H-Purine-2-carbonitrile, 8-(3-amino-1-piperidinyl)-7-(2-butynyl)-1-[(2-cyanophenyl)methyl]-6,7-dihydro-6-oxo-, monohydrochloride (9CI) (CA INDEX NAME)

$$NC$$
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $NH_2$ 
 $CH_2-C$ 
 $CH_2-C$ 
 $CH_2-C$ 

● HCl

RN 635720-26-2 USPATFULL

CN Benzonitrile, 2-[[8-(3-amino-1-piperidinyl)-7-(2-butynyl)-6,7-dihydro-2-methoxy-6-oxo-1H-purin-1-yl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

#### ● HCl

RN 635720-27-3 USPATFULL

CN 1H-Purine-2-carbonitrile, 8-(3-amino-1-piperidinyl)-7-(2-butynyl)-6,7-dihydro-6-oxo-1-(2-phenylethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

## ● HCl

RN 635720-28-4 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-7-(2-butynyl)-1,7-dihydro-2-methoxy-1-(2-phenylethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

#### ● HCl

RN 635720-29-5 USPATFULL

CN 1H-Purine-2-carbonitrile, 8-(3-amino-1-piperidinyl)-7-(2-butynyl)-1-[(4-cyanophenyl)methyl]-6,7-dihydro-6-oxo-, monohydrochloride (9CI) (CA INDEX NAME)

### ● HCl

RN 635720-30-8 USPATFULL

CN Benzonitrile, 4-[[8-(3-amino-1-piperidinyl)-7-(2-butynyl)-6,7-dihydro-2-methoxy-6-oxo-1H-purin-1-yl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

# ● HCl

RN 635720-34-2 USPATFULL

CN 1H-Purine-2-carbonitrile, 8-(3-amino-1-piperidinyl)-7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635720-33-1 CMF C16 H19 N7 O

NC N N N NH2

Me 
$$CH_2-C \equiv C-Me$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635720-36-4 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-7-(2-butynyl)-2-[(1,1-dimethylethyl)thio]-1,7-dihydro-1-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635720-35-3 CMF C19 H28 N6 O S

t-BuS N N N NH2 NH2 
$$\sim$$
 CH2-C  $\sim$  C-Me

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635720-38-6 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-7-(2-butynyl)-1,7-dihydro-2-methoxy-1-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635720-37-5 CMF C16 H22 N6 O2

$$\begin{array}{c|c} \text{MeO} & \text{N} & \text{N} & \text{N} \\ \text{N} & \text{N} & \text{N} & \text{N} \\ \text{Me} & \text{CH}_2\text{--}\text{C} \Longrightarrow \text{C--}\text{Me} \end{array}$$

CRN 76-05-1 CMF C2 H F3 O2

RN 635720-40-0 USPATFULL

CN 6H-Purin-6-one, 8-(3-amino-1-piperidinyl)-7-(2-butynyl)-2-(diethylamino)-1,7-dihydro-1-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 635720-39-7 CMF C19 H29 N7 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 635720-43-3 USPATFULL

CN 1H-Purine-2-carbonitrile, 7-(2-butynyl)-6,7-dihydro-1-methyl-8-[3-(methylamino)-1-piperidinyl]-6-oxo-, monohydrochloride (9CI) (CA INDEX NAME)

NC N N N N NHMe NHMe 
$$CH_2-C = C-Me$$

## ● HCl

RN 635720-45-5 USPATFULL

CN 1H-Purine-2-carbonitrile, 8-(3-amino-1-pyrrolidinyl)-7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \operatorname{NC} & \operatorname{N} & \operatorname{NH}_2 \\ \\ \operatorname{N} & \operatorname{N} & \operatorname{CH}_2 - \operatorname{C} = \operatorname{C-Me} \end{array}$$

### ● HCl

IT 635717-07-6 635723-88-5

(preparation of purinone derivs. as dipeptidylpeptidase IV inhibitors)

RN 635717-07-6 USPATFULL

CN 1H-Purine-2-carbonitrile, 7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)

RN 635723-88-5 USPATFULL

CN 1H-Purine-2-carbonitrile, 7-(2-butynyl)-1-[(2-cyanophenyl)methyl]-6,7-dihydro-6-oxo-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)

IT 635722-55-3P 635722-62-2P 635722-67-7P 635722-85-9P 635722-93-9P 635723-71-6P

635723-77-2P

(preparation of purinone derivs. as dipeptidylpeptidase IV inhibitors)

RN 635722-55-3 USPATFULL

CN 1-Piperazinecarboxylic acid, 4-[2-(aminocarbonyl)-7-(2-butynyl)-6,7-dihydro-1-methyl-6-oxo-1H-purin-8-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 635722-62-2 USPATFULL

CN 1-Piperazinecarboxylic acid, 4-[7-(2-butynyl)-1-[(2-cyanophenyl)methyl]-2-(dimethylamino)-6,7-dihydro-6-oxo-1H-purin-8-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$CH_2$$
 $CH_2$ 
 $CH_2$ 

RN 635722-67-7 USPATFULL

CN 1-Piperazinecarboxylic acid, 4-[6,7-dihydro-6-oxo-7-(phenylmethyl)-1H-purin-8-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 635722-85-9 USPATFULL

CN 1-Piperazinecarboxylic acid, 4-[7-(2-butynyl)-2-cyano-1-[(2-

cyanophenyl)methyl]-6,7-dihydro-6-oxo-1H-purin-8-yl]-, 1,1-dimethylethyl
ester (9CI) (CA INDEX NAME)

$$CH_2$$
 $CH_2$ 
 $CH_2$ 

RN 635722-93-9 USPATFULL

CN Carbamic acid, [1-[7-(2-butynyl)-2-cyano-1-[(2-cyanophenyl)methyl]-6,7-dihydro-6-oxo-1H-purin-8-yl]-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 635723-71-6 USPATFULL

CN 1-Piperazinecarboxylic acid, 4-[7-(2-chlorophenyl)-2-(2-ethoxy-2-oxoethoxy)-6,7-dihydro-1-methyl-6-oxo-1H-purin-8-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 635723-77-2 USPATFULL

CN 1-Piperazinecarboxylic acid, 4-[7-(2-butynyl)-2-cyano-6,7-dihydro-1-methyl-6-oxo-1H-purin-8-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

 $\begin{array}{c|c} & & & & \\ & & & \\ NC & & & \\ N & & & \\ C & & \\ C$ 

L32 ANSWER 15 OF 17 USPATFULL on STN

ACCESSION NUMBER: 93:91634 USPATFULL

TITLE: (4-piperidinylmethyl and -hetero)purines
INVENTOR(S): Janssens, Frans E., Bonheiden, Belgium
Diels, Gaston S. M., Ravels, Belgium

PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Beerse, Belgium (non-U.S.

corporation)

DISCLAIMER DATE: 20080820

RELATED APPLN. INFO.: Division of Ser. No. US 1989-323250, filed on 9 Mar 1989, now patented, Pat. No. US 5041448 which is a

continuation of Ser. No. US 1986-858339, filed on 1 May

1986, now abandoned

NUMBER DATE
PRIORITY INFORMATION: GB 1985-15934 19850624

DOCUMENT TYPE: Utility FILE SEGMENT: Granted

PRIMARY EXAMINER: Rizzo, Nicholas S. LEGAL REPRESENTATIVE: Metz, Charles J.

NUMBER OF CLAIMS: 6
EXEMPLARY CLAIM: 1
LINE COUNT: 2450

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB (4-Piperidinylmethyl and -hetero)purines having antihistaminic properties and being useful agents in the treatment of allergic diseases.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 116062-65-8P

(preparation and alkylation of)

RN 116062-65-8 USPATFULL

CN 6H-Purin-6-one, 7-[(4-fluorophenyl)methyl]-1,7-dihydro-8-(4-piperidinylamino)-, dihydrobromide (9CI) (CA INDEX NAME)

### •2 HBr

IT 116062-74-9P 116062-92-1P 116063-06-0P

116063-46-8P

(preparation of, as antiallergic agent)

RN 116062-74-9 USPATFULL

CN 6H-Purin-6-one, 8-[[1-[(2,3-dihydro-1,4-benzodioxin-2-y1)methyl]-4-piperidinyl]amino]-7-[(4-fluorophenyl)methyl]-1,7-dihydro-(9CI) (CAINDEX NAME)

RN 116062-92-1 USPATFULL

CN 6H-Purin-6-one, 7-[(4-fluorophenyl)methyl]-1,7-dihydro-8-[[1-[2-(4-methoxyphenyl)ethyl]-4-piperidinyl]amino]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} H & N - CH_2 - CH_2 \\\hline N & N - CH_2 - CH_2 \\\hline \end{array}$$

RN 116063-06-0 USPATFULL

CN 4H-Pyrido[1,2-a]pyrimidin-4-one, 3-[2-[4-[[7-[(4-fluorophenyl)methyl]-6,7-dihydro-6-oxo-1H-purin-8-yl]amino]-1-piperidinyl]ethyl]-2-methyl- (9CI)

### (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} & \text{N} \\ & \text{H} & \text{N} & \text{CH}_2 - \text{CH}_2 - \text{CH}_2 \\ & \text{N} & \text{N} - \text{CH}_2 \\ & \text{O} & \text{F} \end{array}$$

RN 116063-46-8 USPATFULL

CN 6H-Purin-6-one, 7-[(4-fluorophenyl)methyl]-1,7-dihydro-8-[(1-methyl-4-piperidinyl)amino]- (9CI) (CA INDEX NAME)

L32 ANSWER 16 OF 17 USPATFULL on STN

ACCESSION NUMBER: 91:66801 USPATFULL

TITLE: (4-piperidinylmethyl and -hetero) purines
INVENTOR(S): Janssens, Frans E., Bonheiden, Belgium

Diels, Gaston S. M., Ravels, Belgium

PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Beerse, Belgium (non-U.S.

corporation)

APPLICATION INFO.: US 1989-323250 19890309 (7)

RELATED APPLN. INFO.: Continuation of Ser. No. US 1986-858339, filed on 1 May

1986, now abandoned

DOCUMENT TYPE: Utility FILE SEGMENT: Granted

PRIMARY EXAMINER: Rizzo, Nicholas S. LEGAL REPRESENTATIVE: Metz, Charles J.

LEGAL REPRESENTATIVE: Metz
NUMBER OF CLAIMS: 6
EXEMPLARY CLAIM: 1
LINE COUNT: 2399

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB (4-Piperidinylmethyl and -hetero)purines having antihistaminic properties and being useful agents in the treatment of allergic diseases.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 116062-65-8P

(preparation and alkylation of)

RN 116062-65-8 USPATFULL

CN 6H-Purin-6-one, 7-[(4-fluorophenyl)methyl]-1,7-dihydro-8-(4-piperidinylamino)-, dihydrobromide (9CI) (CA INDEX NAME)

### •2 HBr

IT 116062-74-9P 116062-92-1P 116063-06-0P

116063-46-8P

(preparation of, as antiallergic agent)

RN 116062-74-9 USPATFULL

CN 6H-Purin-6-one, 8-[[1-[(2,3-dihydro-1,4-benzodioxin-2-yl)methyl]-4-piperidinyl]amino]-7-[(4-fluorophenyl)methyl]-1,7-dihydro-(9CI) (CA INDEX NAME)

RN 116062-92-1 USPATFULL

CN 6H-Purin-6-one, 7-[(4-fluorophenyl)methyl]-1,7-dihydro-8-[[1-[2-(4-methoxyphenyl)ethyl]-4-piperidinyl]amino]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} H & N - CH_2 - CH_2 \\ \hline N & N - CH_2 - CH_2 \\ \hline \end{array}$$

RN 116063-06-0 USPATFULL

CN 4H-Pyrido[1,2-a]pyrimidin-4-one, 3-[2-[4-[[7-[(4-fluorophenyl)methyl]-6,7-

dihydro-6-oxo-1H-purin-8-yl]amino]-1-piperidinyl]ethyl]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & \\ H & & \\ N & & \\ N & & \\ N & & \\ O & & \\ \end{array}$$

116063-46-8 USPATFULL RN

6H-Purin-6-one, 7-[(4-fluorophenyl)methyl]-1,7-dihydro-8-[(1-methyl-4-CNpiperidinyl)amino] - (9CI) (CA INDEX NAME)

L32 ANSWER 17 OF 17 USPATFULL on STN

ACCESSION NUMBER:

91:30490 USPATFULL

TITLE:

2-aminopyrimidinone derivatives

INVENTOR(S):

Janssens, Frans E., Bonheiden, Belgium Kennis, Ludo E. J., Turnhout, Belgium Sommen, Francois M., Wortel, Belgium

Dierckx, Ann C. J., Kasterlee, Belgium

PATENT ASSIGNEE(S):

Janssen Pharmaceutica N.V., Beerse, Belgium (non-U.S.

corporation)

KIND NUMBER DATE 19910416 US 5008268 PATENT INFORMATION: US 1989-456391 19891226 (7) APPLICATION INFO.:

> NUMBER DATE

PRIORITY INFORMATION:

19890109 GB 1989-380

DOCUMENT TYPE:

Utility

FILE SEGMENT:

Granted

PRIMARY EXAMINER: LEGAL REPRESENTATIVE: Ford, John M.

NUMBER OF CLAIMS: 18

Metz, Charles J.

EXEMPLARY CLAIM:

1,7

LINE COUNT:

1600

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB

2-Amino-pyrimidininone derivatives possessing antihistaminic and serotonin-antagonistic properties. Compositions containing these compounds as the active ingredient and a method of treating subjects from allergic diseases.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 131264-36-3P

(preparation of, as antihistaminic and antiserotoninergic)

RN 131264-36-3 USPATFULL

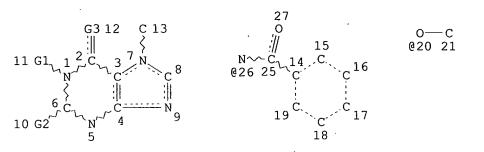
CN 1,2,4-Triazolo[4,3-a]pyrimidin-5(1H)-one, 6-[2-[4-[[7-[(4-fluorophenyl)methyl]-6,7-dihydro-6-oxo-1H-purin-8-yl]amino]-1-piperidinyl]ethyl]-1,3,7-trimethyl- (9CI) (CA INDEX NAME)

FILE 'HOME' ENTERED AT 16:37:30 ON 12 MAY 2005

=>



0 @22



S—C @23 24

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VAR G2=H/C/N/20/22/23
VAR G3=O/S
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CONNECT IS E1 RC AT 22
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

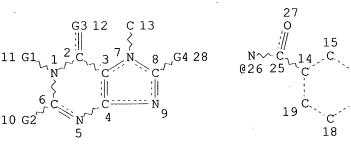
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STEREO ATTRIBUTES: NONE

L12 L20

C @29

35177 SEA FILE=REGISTRY SSS FUL L9 STR



 $N \sim G6 \sim N$ 

@31 32 33

CH~G5~Cb N~G7~Cb @34 35 36 @37 38 39

O--- C

@20 21

S---C

@23 24

CH~G5~N N~G8 43 44 6 45

N @30

VAR G1=C/NH2/26/H

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VAR G2=H/C/N/20/23

VAR G3=O/S

VAR G4=29/30/31/34/37/40/48

REP G5=(0-3) CH

REP G6=(1-4) CH

REP G7 = (0-4) CH

REP G8 = (0-2) CH

REP G9=(1-3) C

NODE ATTRIBUTES:

NSPEC IS RC AT 13 NSPEC IS R AT 29

NSPEC IS R AT 30

DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

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RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 47

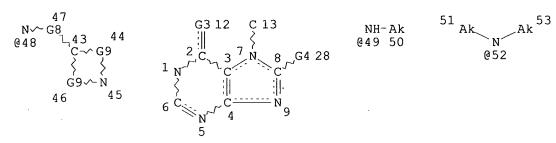
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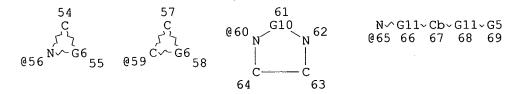
L22

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456 SEA FILE=REGISTRY SUB=L12 SSS FUL L20

L24 STR





Page 1-A

CH-G15~G5

088 89 90

Page 2-A VAR G3=O/S

VAR G4=56/59/60/65/70/75/48/83/84/88

VAR G5=NH2/49/52

REP G6=(1-9) C

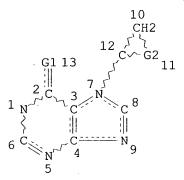
11110 1 250 212111 (USP10)

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REP G9 \approx (1-3) C
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REP G11 = (0-4) C
REP G12=(0-3) C
REP G13 = (1-4) CH
REP G14 = (0-1) CH
REP G15=(1-3) CH
NODE ATTRIBUTES:
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                        13
CONNECT IS E1
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                        50
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                        51
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                        53
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                      67
        IS SAT
                     72
GGCAT
                 AT
DEFAULT ECLEVEL IS LIMITED
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RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 60

STEREO ATTRIBUTES: NONE L26 STR



VAR G1=O/S REP G2=(1-9) CH2 NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE L27 STR

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G2@28

VAR G1=O/S
VAR G2=NH2/14/17/19
REP G3=(0-3) C
VAR G5=NH2/14/17
VPA 28-22/27/23 U
NODE ATTRIBUTES:
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CONNECT IS E1 RC AT 16
CONNECT IS E1 RC AT 18
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE

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445 ANSWERS

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SET LINE LOGIN

SET DETAIL LOGIN



D SCAN SEL RN

L2

L3

L4

L5

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OR 75-16-1/BI OR 75-31-0/BI OR 79463-77-7/BI)

82 SEA ABB=ON L2 AND NR>1 D SCAN

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FILE 'CAPLUS' ENTERED AT 15:09:48 ON 12 MAY 2005

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E US2003-636088/AP, PRN 25

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SEL RN

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rs
L9
                STR L7
L10
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L11
             50 SEA SSS SAM L9
L12
          35177 SEA SSS FUL L9
                SAVE TEMP L12 BER088FULL/A
L13
                STR L9
L14
              2 SEA SUB=L12 SSS SAM L13
                D SCAN
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                SAVE TEMP L15 BER088SUB/A
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L18
              8 SEA ABB=ON L15
L19
              8 DUP REM L18 (O DUPLICATES REMOVED)
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                     ANSWERS '6-8' FROM FILE USPATFULL
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                D OUE L12
L20
                STR L9
L21
             24 SEA SUB=L12 SSS SAM L20
            456 SEA SUB=L12 SSS FUL L20
L22
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L23
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STR L20

L24

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L26 STR L25,
L27 STR L26
L28 27 SEA SUB=L22 SSS SAM (L24 NOT (L26 OR L27))
L29 445 SEA SUB=L22 SSS FUL (L24 NOT (L26 OR L27))
SAVE TEMP L29 BER047SUB/A
L30 ANALYZE L29 1- LC : 5 TERMS
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FILE 'REGISTRY' ENTERED AT 16:36:06 ON 12 MAY 2005 D STAT QUE L29

FILE 'HOME' ENTERED AT 16:37:30 ON 12 MAY 2005

D STAT QUE L29

D STAT QUE L29

FILE HOME

FILE CAPLUS

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FILE COVERS 1907 - 12 May 2005 VOL 142 ISS 20 FILE LAST UPDATED: 11 May 2005 (20050511/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.  $\begin{tabular}{ll} \hline \end{tabular}$ 

## FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 11 MAY 2005 HIGHEST RN 850303-40-1 DICTIONARY FILE UPDATES: 11 MAY 2005 HIGHEST RN 850303-40-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

FILE STNGUIDE
FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: May 6, 2005 (20050506/UP).

FILE USPATFULL

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 12 May 2005 (20050512/PD)

FILE LAST UPDATED: 12 May 2005 (20050512/ED)

HIGHEST GRANTED PATENT NUMBER: US6892391

HIGHEST APPLICATION PUBLICATION NUMBER: US2005102725

CA INDEXING IS CURRENT THROUGH 12 May 2005 (20050512/UPCA)

ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 12 May 2005 (20050512/PD)

REVISED CLASS FIELDS (/NCL) LAST RELOADED: Feb 2005

USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2005

USPAT2 is now available. USPATFULL contains full text of the >>> <<< original, i.e., the earliest published granted patents or >>> <<< applications. USPAT2 contains full text of the latest US >>> <<< >>> publications, starting in 2001, for the inventions covered in <<< USPATFULL. A USPATFULL record contains not only the original <<< >>> >>> published document but also a list of any subsequent <<< publications. The publication number, patent kind code, and <<< >>> >>> publication date for all the US publications for an invention <<< >>> are displayed in the PI (Patent Information) field of USPATFULL <<< >>> records and may be searched in standard search fields, e.g., /PN, <<< >>> /PK, etc. <<< USPATFULL and USPAT2 can be accessed and searched together >>> <<< >>> through the new cluster USPATALL. Type FILE USPATALL to <<< >>> enter this cluster. <<< >>> <<< >>> Use USPATALL when searching terms such as patent assignees, <<< ·>>> classifications, or claims, that may potentially change from <<< the earliest to the latest publication. <<<

This file contains CAS Registry Numbers for easy and accurate substance identification.

## FILE TOXCENTER

FILE COVERS 1907 TO 10 May 2005 (20050510/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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New CAS Information Use Policies, enter HELP USAGETERMS for details.

TOXCENTER has been enhanced with new files segments and search fields. See  ${\tt HELP}$  CONTENT for more information.

TOXCENTER thesauri in the /CN, /CT, and /MN fields incorporate the MeSH 2005 vocabulary. See http://www.nlm.nih.gov/mesh/ and http://www.nlm.nih.gov/pubs/techbull/nd04/nd04\_mesh.html for a description of changes.

